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PROGRAM PREGA PIVOTAL REGRESSION ANALYSIS OF GAMMA-RAY  
SPECTRA FROM NAI(T. (U) NAVAL RESEARCH LAB WASHINGTON  
DC G W PHILLIPS ET AL. 06 APR 84 NRL-MR-5275

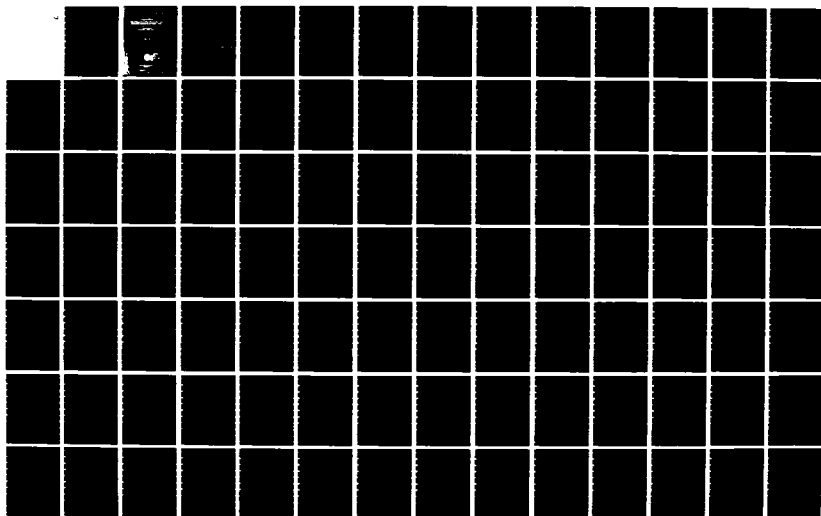
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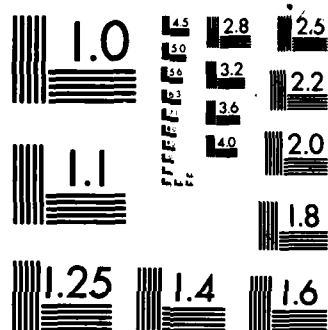
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<p><b>A</b></p> <p>Program PREGA was developed at NRL to perform a fast and efficient regression analysis of a gamma-ray spectrum from an unknown source, taken with a NaI(Tl) detector. The analysis determines the best subset from a library of standard spectra to use in fitting the data. Output at each step includes relative intensities and uncertainties for each standard used in the fit, plus the partial F statistic for significance of each library element. Final output includes an analysis of variance (ANOVA) table, distribution of residuals, location of largest residuals, distribution of runs of consecutive residuals with the same sign, and the location of largest runs. The program was written for the Nuclear Data ND6620 computer and has been transferred to VAX II/780.</p>				
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**11. TITLE (Include Security Classification)**

**PROGRAM PREGA — Pivotal Regression Analysis of Gamma-Ray Spectra from NaI(Tl) Detectors  
for the ND6620 Computer**

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Program PREGA  
Pivotal Regression Analysis  
of Gamma-Ray Spectra from  
NaI(Tl) Detectors  
for the ND6620 Computer

## 1. INTRODUCTION

Gamma-ray pulse-height spectra from NaI(Tl) detectors often contain few or no discernable peaks due to the source of interest, as a result of the poor intrinsic resolution of these detectors and a predominance of background gamma rays. Even after background subtraction, the resulting spectrum is often of too poor a quality to reveal characteristic peaks. Thus, one cannot do a peak analysis such as is usually performed on gamma-ray spectra from high-resolution germanium diode detectors (see Ref. 1).

However, there is often sufficient information contained in such spectra in the overall spectral shape to identify the source of the gamma rays by comparison to a library of standard source shapes. The situation becomes more complicated when the spectrum may be due to a superposition of gamma-ray spectra from two or more sources. To determine the relative contributions of the individual sources it is necessary to do a multiple least-squares fit of the unknown source spectrum to a library of standard source spectra using regression analysis techniques.

The ALPHA-M program was developed at Oak Ridge<sup>2</sup> to perform such a fit and calculate the concentrations of each of the standards in the unknown.

However, if there are more than a very few standards in the library, such a procedure often gives an ambiguous result, due to correlations between library spectra. In such a case, it is necessary to do a systematic search for the subset of library standards which gives the best fit to the unknown spectrum. Program PREGA was developed at NRL to efficiently perform this search for the best subset. It works in one of two optional modes.

The first mode is similar to standard stepwise regression analysis methods. It begins with a subset containing only background, and performs a least-squares fit for the intensity of the background in the unknown spectrum. It then calculates the correlation of the residual spectrum, not accounted for by background, with each of the remaining standards in the library. That standard with the largest correlation is added to the fitting subset and a new least-squares fit is performed. This continues until no remaining standards are significantly correlated with the residuals.

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The second mode begins with a fit to the full library. From the results of this fit a test set of library members most correlated with the unknown spectrum is selected. Additional library members are then pivoted in and out of the test set, depending on their correlation with the residuals, until the subset which gives the best significant fit is obtained.

PREGA begins by calculating the matrix of cross-correlations of the library members with each other and with the unknown spectrum. It then operates on this matrix using a method by Garside<sup>3</sup> to obtain the quantities of interest in the fit with a minimum of mathematical manipulations. At no time is it necessary to do a complete matrix inversion, and individual library members can be pivoted into and out of the fit quickly and simply. This method is thus tailor-made for either the stepwise mode or the full library mode of PREGA.

The program PREGA is implemented as an extensive modification of the program NAI supplied by Nuclear Data, Inc.<sup>4</sup> and runs on the Nuclear Data ND 6620 system. It is written in DEC RT-11 FORTRAN and is currently being adapted to run on the Digital Equipment Corporation VAX 11/780.

## 2. SETUP FOR ANALYSIS

### Preparation of Library

Library spectra should be taken for each source of interest under conditions as close as possible as those under which the unknown spectrum is taken. Backscattering of gamma rays by nearby materials can affect the shape of the spectrum as can attenuation due to intervening materials between the source and detector. This results in removal of counts from the full-energy peaks and the addition of counts with lower energy due to scattered gamma rays.

Background spectra taken before and after each library spectrum should be normalized by counting time and subtracted from the library spectrum. An energy calibration must be determined either from known peaks in the library or background spectra, or from a calibration source spectrum taken before and after each library spectrum. Program PKANAL is included in the PREGA package and may be used to determine the position of the peaks. At least two peaks are needed, well separated in energy, to determine a linear calibration of peak energy  $E$  versus channel number  $I$  in the form

$$E(I) = E_0 + I \cdot E_1.$$

If more than two peaks are available a linear least squares fit can be used to determine the offset  $E_0$  and slope  $E_1$ . These should be recorded with each library spectrum along with source type, configuration, strength, range, attenuation and any other pertinent information.

### Preparation of Background

A background spectrum should be taken as close as possible in time and other conditions to the unknown, preferably immediately before and after. An energy calibration should be obtained in the same manner as for the

library spectra. Program GSHIFT can then be used to shift the slope and offset of each library member to match the slope and offset of the unknown spectrum. PREGA has the option of subtracting the background from the unknown before fitting. Nevertheless, the background spectrum should be included in the library, because background intensity changes could lead to over or under subtraction. If this happens, a negative intensity may result for the background. To allow for this PREGA has the option of not allowing the background to be pivoted out. (A negative intensity for any other library member is generally not physically allowable and should be rejected).

#### Preparation for PREGA

The library to be used in the fit is specified interactively in the program SEDIT. The standard name, file name, counting time and half-life activity are specified for each library member. A background spectrum, which may be subtracted from each library member, must be specified although this is generally not used.

The unknown and its background are specified interactively in the program UEDIT. This also allows the user to select various options to be used in the fit and to select which of the library members will be used. The information entered by the user in SEDIT and UEDIT are written to control files which are used by PREGA to perform the fit. Thus PREGA requires no direct input from the user and can be run as a batch job if desired. Output is usually to a file which can be listed later on the lineprinter.

#### Selection of Mode

If only one or two library members are expected to be present together in the unknown, the stepwise mode of PREGA is usually more efficient than the mode which begins by using the entire library in the fit. If multiple library members may be present, it is usually best to run both modes. They will generally, but not always, agree on the subset of library members which give the best fit. In cases where they do not agree, correlations between library members or linear combinations of library members will be found to cause ambiguities in the fit. Enough information is printed out at each step for the analyst to determine which library members are causing the ambiguity. They can either be eliminated from the library or accepted as doubtful contributions to the unknown spectrum.

### 3. ALGORITHMS

#### Partial F Test

The criterion used for selection or rejection of library members at each step is given by the partial F-test statistic  $F_p$  defined in Chapter 4. For convenience, this is converted to an equivalent normally distributed parameter  $X(F)$  which gives the value of  $F_p$  in standard deviations (sigma units). This is compared to a threshold  $F_0$  usually set at 2.5 sigma.

## Full PREGA

The full PREGA algorithm begins with the fit to the complete library and selection of the trial subset C. It then goes directly to the regression on the trial subset C. PREGA then pivots library elements out (backward step) and in (forward step) successively, based on the partial F-values, until a best fit is found. The full PREGA algorithm proceeds as follows:

1. Do the fit to the complete library L.
2. Let the trial subset C include all library elements I with a relative intensity  $B_I$  and error  $\sigma_I(B)$  such that
$$B_I/\sigma_I(B) > 1.$$
3. Let E be the set containing all library elements included in the fit at each step. Initially let  $E = C$ .
4. Let D be the set of elements not in the fit at the beginning of step 6, below. Initially let  $D = 0$  (empty set).
5. Backward Pivot: to check for removal of library elements from subset E.
  - a. Let  $C = E$ .
  - b. Calculate partial F to remove,  $F_p(I)$ , for all library elements I in C.
  - c. Let  $F_p(J) = \min F_p(I)$ , for all I in C, and convert to  $X(F)_J$  in sigma units.
  - d. IF:  $X(F)_J < F_0$ ,  
THEN: remove J, let  $E = E - J$ ;  
ELSE: continue.
  - e. IF:  $E = L - D$ , (no change in trial subset)  
THEN: end regression (go to 7);  
ELSE: continue.
6. Forward Pivot: to check for addition of library elements not in C during step 5.
  - a. Let  $D = L - C$
  - b. Calculate partial F to include,  $F_p(I)$ , for all library elements I in D.
  - c. Let  $F_p(J) = \max F_p(I)$ , for all I in D, and convert to  $X(F)_J$  in sigma units.

- d. IF:  $X(F)_J > F0$ ,  
 THEN: include J, let  $E = E+J$ ;  
 ELSE: continue.
- e. IF:  $E = C$ , (no change in trial subset)  
 THEN: end regression (go to 7);  
 ELSE: repeat pivots, go to 5.
- 7. End regression: do analysis of variance, calculate residuals and runs, and print out results.

### Stepwise PREGA

The stepwise PREGA mode is implemented as an option of program PREGA. It is run by setting the Background Regression (BR) parameter in UEDIT to 1: trial set = background only. The stepwise mode proceeds as follows:

1. Begin regression with fit to background only.
2. Let the trial subset  $C = (\text{background})$ .
3. Initially let  $E = C$ .
4. Go to the forward pivot (step 6) of the full PREGA mode and proceed from there on as in the full PREGA.

### 4. FORMULAS AND DEFINITIONS

1. Let  $Y$  be the vector of the observed source data spectrum,

$$Y = \{y(1), y(2), \dots, y(N)\},$$

and let  $X_I$  be a similar vector for the spectrum of library element  $I$ .

2. Define the augmented cross-product matrix  $S_L$  of dimension  $K$ , where the number of library elements is  $K-1$ , by

$$S_L = \{S_{IJ}\} \text{ for } I, J = 1, \dots, K$$

where

$$S_{IJ} = (X_I \cdot S_J), \text{ for } I, J=1, \dots, K-1$$

$$S_{IK} = (X_I \cdot Y)$$

$$S_{KJ} = (Y \cdot X_J)$$

$$S_{KK} = (Y \cdot Y),$$

and the dot product

$$(X_I \cdot X_J) \triangleq \sum_{r=1}^N w(r) x_I(r) x_J(r)$$

The weights  $w(r)$  are calculated by the inverse Poisson variances of the data  $y(r)$ .

3. The least squares solution for

$$Y = B X + \epsilon,$$

where  $\epsilon$  is the vector of random errors in the data, is given by

$$B = (X \cdot X)^{-1} (X \cdot Y)$$

where  $B$  is the vector of coefficients of the library elements in the fit,

$$B = \{B_1, \dots, B_{k-1}\}.$$

4. The residual sum of squares is given by

$$\begin{aligned} \text{RSS} &= (Y - BX)^T (Y - BX) \\ &= (Y \cdot Y) - (X \cdot Y)^T (X \cdot X)^{-1} (X \cdot Y). \end{aligned}$$

5. The results of a regression of  $Y$  on a subset  $C$  of the library  $L$  can be completely determined from the matrix  $S_C^*$  obtained by successive pivots  $\phi$  on the matrix  $S_L$ , for each library element in  $C$ . The pivot operation used in PREGA is described by Garside.<sup>3</sup> The results for  $N$  data points and  $P$  elements  $I$  in  $C$  are

$$B_I = S_{IK}^*$$

$$\text{RSS}_C = S_{KK}^*$$

$$\hat{\sigma}_C^2 = \text{RSS}_C / (N - P)$$

$$\sigma_I(B)^2 = S_{II}^* \hat{\sigma}_C^2$$

6. The partial F-test<sup>4</sup> to remove library element I from C is given, for  $H = C-I$ , by

$$\begin{aligned} F_p^-(I) &= (RSS_H - RSS_C)/(RSS_C/(N-P)) \\ &= B_I^2/\sigma_I(B)^2 \\ &= (N-P)(S_{IK}^*)^2/(S_{II}^* S_{KK}^*) \end{aligned}$$

then

$$RSS_H = RSS_C (1 + F_p^-(N-P)).$$

7. The partial F test to include library element J not in C is given, for  $G = C+J$ , by

$$F_p^+(J) = (RSS_C - RSS_G)/(RSS_G/(N-P-1))$$

where

$$RSS_G = RSS_C(1 - R_{JK.C}^2)$$

and the partial correlation coefficient of J and K given C is just<sup>6</sup>

$$R_{JK.C}^2 = (S_{JK}^*)^2/(S_{JJ}^* S_{KK}^*).$$

8. An approximate normal transformation for F with D,1 degrees of freedom is used,\*

$$X(F) \approx \sqrt{F} (1 - 1/4D)/(1 - F/2D)^{1/2}$$

(note that for  $D \gg 1$  and  $D \gg F$  then  $X \approx \sqrt{F}$ ).

9. An approximation for the probability of obtaining a random value greater than X is used,\*

$$Q(X) \approx Z(X)(a_1 t + a_2 t^2 + a_3 t^3)$$

where

$$Z(X) = \exp(-X^2/2)/(2\pi)^{1/2},$$

$$t = 1/(1 + pX),$$

and

$$\begin{aligned} a_1 &= .436184, a_2 = -.120168, \\ a_3 &= .937298, p = .33267. \end{aligned}$$

\*See the "Handbook of Mathematical Functions," edited by M. Abramowitz and I.A. Stegun, Dover Publications, New York (1965).

## 5. PROGRAM PKANAL

### Operation

Program PKANAL reads in data from ND spectral files and calculates a background, peak positions, width and area for selected regions.

### Language

The program is written in DEC RT11 FORTRAN and runs on the Nuclear Data ND6620 computer under the MIDAS operating system.

### Inputs

Diskfile	logical unit (LU) 8, spectral data in ND format
Keyboard	LU 5, operator inputs first and last channels for up to 20 regions followed by one or more filenames containing spectra to be analyzed
Outputs	LU6, table of results for each spectrum

### Input Variables

Record 1a,... JL, JR	lower and upper limits of each region to be analyzed, one pair of limits per record up to a maximum of twenty (20), terminated with a double carriage return
Record 2a,...	filenames for spectra to be analyzed, one per record, terminated with a double carriage return

### Lineprinter Output

<u>Heading</u>	<u>Contents</u>
REGION LIMITS	input limits (JL,JR) for region
PEAK LIMITS	limits determined by the program for the peak
HEIGHT	maximum peak height above background
AREA	net peak area above background
BKGD	background area beneath the peak
CENTROID	calculated peak position (center of gravity)
VARIANCE	calculated variance about centroid
FWHM	peak full width at half maximum
ENERGY	calibrated energy of centroid position

### Subroutines Called

FREEFM	free field input routine
GET	reads spectrum from ND spectral files
PEAKNL	does peak analysis for each region

## 6. PROGRAM GSHIFT

### Operation

Program GSHIFT reads in a spectrum and its energy calibration from disk, performs a specified gain shift and zero offset, and writes the shifted spectrum and its calibration back to disk.

### Language

The program is written in DEC RT11 FORTRAN and runs on the Nuclear Data ND6620 computer under the MIDAS operating system.

### Inputs

Diskfile	logical unit (LU) 8, spectral data in ND format
Keyboard	LU5, operator inputs filenames and selects new gain or desired shift

### Outputs

Diskfile	LU8, shifted spectrum in ND format
CRT	LU5, prompts to operator, energy calibration from header, etc.

### Input from Keyboard

<u>Rec.</u>	<u>Prompt</u>	<u>Response</u>
1.	FILENAME FOR SPECTRUM	FILE.ELEMENT (for input spectrum)
2a.	ENERGY CALIB. FROM HEADER GIVES . . . . USE THIS . . .	YES (go to 3a.), <u>or</u> NO (go to 2b), (default = NO)*
2b.	ENTER OLD SLOPE, OFFSET	slope, offset (for calibration of input spectrum)

- |     |                                     |   |
|-----|-------------------------------------|---|
| 3a. | TO GET NEW SLOPE<br>AND OFFSET. . . | FILE.ELEMENT<br>(spectrum with desired slope and<br>offset in header, go to 4),<br>(default, go to 3b)* |
| 3b. | ENTER NEW SLOPE,<br>OFFSET          | slope, offset<br>(for desired calibration,<br>go to 4),<br>(default, go to 3c)*                         |
| 3c. | ENTER GAIN, ZERO<br>SHIFT           | desired gain, zero shift  |
| 4.  | FILENAME FOR<br>OUTPUT SPECTRUM     | FILE.ELEMENT  |

\*immediate carriage return gives default values

#### Subroutines Called

GET	reads spectrum and energy calibration from ND spectral file
FREEFM	free field input routine
REGAIN	performs gain and zero shift
RECHAN	restores proper channel offset after call to REGAIN
PUT	writes spectrum and energy calibration to ND spectral file

## 7. PROGRAM PREGA

### Operation

Program PREGA performs a stepwise or pivotal regression analysis in order to fit a data spectrum to the "best" subset of a library consisting of a background spectrum and several characteristic source spectra. The program is essentially a modification to the Nuclear Data Inc. ND6600 NAI Data Reduction Package,<sup>5</sup> designed to make analysis more efficient for the user. Therefore, the basic package architecture used by Nuclear Data Inc. is still retained as far as program input, file structure and logical units used is concerned. The general flow of PREGA is given in the flow chart in Fig. 1. A more detailed flow chart is given in Appendix B.

### Language

The program is written in DEC RT11 FORTRAN and runs on the Nuclear Data ND6620 computer under the MIDAS operating system.

The program PREGA does not accept information directly from the user to perform its calculations; parameters and calculation options are entered through, and edited by, the editor programs SEDIT and UEDIT. All spectral data acquired by the user are stored on disk files and automatically read by PREGA; the user has only to indicate, via the editor programs, the locations of the spectral data.

For the purposes of this discussion, all input data may be grouped into six categories:

- (1) spectral data
- (2) individual library standard parameters
- (3) all library standard parameters and calculation options
- (4) sample spectrum parameters
- (5) sample background parameters and calculation options
- (6) weighting factor calculation options

On the following pages are listed all the necessary input data for the PREGA Program; where user options are available, they are mentioned.

For a more complete description of the input data, the user is referred to the section containing the listings and descriptions of the programs UEDIT and SEDIT. The actual use of UEDIT and SEDIT by PREGA is referred to in the section on software organization.

#### (1) Spectral Data

Gamma-ray spectra are acquired by the user in the laboratory and written on a disk file in spectral data format.

#### (2) Individual Library Standard Parameters

- a. (standard number: 1 to 10 assigned by SEDIT in sequential order)

- b. standard name: 8 characters maximum
- c. location of individual standard spectrum on disk file LU-8:  
FILE.ELEMENT(,DEVICE)
- d. half-life
- e. half-life units: Y,D,H,M or S
- f. counting time in seconds
- g. activity (concentration): usually set to 1, or may be set to convenient units

(3) All Library Standard Parameters and Calculation Options

- a. number of channels per standard: maximum 512
- b. initial channel number
- c. final channel number
- d. location of background spectrum on disk file LU-8:  
FILE.ELEMENT(,DEVICE)
- e. counting time for background spectrum, in seconds
- f. background subtracted from spectrum: Yes or No?
- g. number of isotopes used from library
- h. printout order of library standards
- i. library standard rejection coefficient; usually  $8/\sigma < 1$
- j. rejection coefficient applied Yes or No?
- k. F-test rejection coefficient; usually set to 2.5

(4) Sample Spectrum Parameters

- a. location of sample spectrum on disk file LU-8:  
FILE.ELEMENT(,DEVICE)
- b. counting time, in seconds
- c. volume reduction factor; usually set = 1
- d. decay time, in seconds; set = 1
- e. result multiplication factor; usually set = 1

(5) Sample Background Parameters and Calculation Options

- a. location of sample background spectrum on disk file LU-8:  
FILE.ELEMENT(,DEVICE)
- b. background supplied: Yes or No
- c. is background to be subtracted from the sample spectrum Yes or No
- d. counting time of background spectrum, in seconds

(6) Weighting Factor Calculation Options

- a. How determined; user has 2 options:
  - option 1: based on original spectral counts and held constant
  - option 2: based on least-squares spectrum counts
- b. weighting factor calculation: user has 3 options  
( $p_i$  = weighting factor,  $y_i$  = sample counts,  $b_i$  = normalized bkg counts)
  - option 1:  $p_i = 1/y_i$
  - option 2:  $p_i = 1/(y_i + b_i)$
  - option 3:  $p_i = 1$

## Outputs

The output device, usually a line printer, prints out the following items in the order indicated: (see examples in Appendix A).

- (1) sum of standards
- (2) sample spectrum counts in each channel
- (3) sum of background and sample counts
- \* (4) "BACKGROUND NOT INCLUDED AS A STANDARD"
- \* (5) "PIVOT ON BACKGROUND PERMITTED"
- (6) correlation matrix
- \* (7) "STARTING ANALYSIS WITH TRIAL SET=BACKGROUND ONLY"
- (8) Result of current regression
- (9) Final Result
- (10) LLNL R-STATISTIC
- (11) Final Statistics for eliminated standards
- (12) residuals/standard deviations per channel
- (13) suspicious channels
- (14) Distribution of residuals
- (15) Distribution of Runs
- (16) locations and sizes of large runs

\*These items are intended as visual flags in the output for the analyst.

### (1) "SUM OF STANDARDS"

For each standard nuclide in the complete library, the program gives the total number or counts in all channels recorded during the counting time of the radionuclide. These sums are printed out in the same order as the nuclides appear in the library. For the example shown in Appendix A, the complete library contained five (5) standards. In fitting the sample spectrum only four (4) of these standards are actually used. This is the last stage of the program in which the complete library is handled. All subsequent calculations only use the library standards (in the order in which they are listed in variable OR) given in the program UEDIT.

### (2) "SAMPLE SPECTRUM"

On the first line is printed the disk file location (LU-8) of the sample spectrum FILE.ELEMENT(,DEVICE). The sample counts minus the background counts for each channel are then printed. The background counts are multiplied by the ratio of the counting time of the sample counting time of the background to correct for any differences in counting times. The printout should be read horizontally from left to right.

### (3) "BACKGD SUM" and "SAMPLE SUM"

These are the background and sample counts in each channel (see "SAMPLE SPECTRUM" listed above) summed from the initial channel for computation to the final channel for computation. See page 36, program lines 129 and 134.

(4) "BACKGROUND NOT INCLUDED AS A STANDARD"

This is an output flag that is printed only when the background is not included as one of the selected library standards. **\*\*NOTE\*\*** For this flag to be functional the background spectrum must be standard No. 1 in the complete library list. The user is referred to the section on the program SEDIT.

(5) "PIVOT ON BACKGROUND PERMITTED"

This flag is output when the variable BP in UEDIT is set equal to one ( $BP = 1$ ). It means that the user wants to allow the program to perform pivot operations on the background if the calculation allows them. **\*\*NOTE\*\*** This flag requires the background spectrum to be standard No. 1 in the full library (see SEDIT).

(6) "CORRELATION MATRIX"

This matrix is calculated to show the correlation of the user chosen set of standards with themselves and the sample. The standards are output in the order given by the variable OR in UEDIT. The sample always occupies the last row and column of the matrix.

(7) "STARTING ANALYSIS WITH TRIAL SET = BACKGROUND ONLY"

This flag is output when the user wishes to begin the regression with the trial set chosen to be only the background spectrum (UEDIT variable  $BR = 1$ ). In this case PREGA executes in a manner similar to a step-wise regression (STREGA). **\*\*NOTE\*\*** This option flag requires that the background spectrum is standard No. 1 in the full library set (see SEDIT).

(8) Results of current regression

This section of output contains several pieces of information. These are:

- a) A title line stating the type of regression or pivot operation just completed;
- b) The degrees of freedom, Regression Sum of Squares (RSS) and Mean Sum of Squares (MSR);
- c) The name of the standard and its relative concentration and standard error;
- d) The partial F-value to remove and associated Q-value and x-value, and the new MSR for each standard.
- e) If the next operation to be performed is a forward pivot, the name, partial F to add and associated Q- and x-values, the square root of the partial correlation coefficient,  $RHO$ , and the new MSR, are output for each standard being considered.

## (9) FINAL RESULT

This section of output is broken down as follows:

### a) "FIT"

The "FIT" is the reduced  $\chi^2$  statistic and gives an overall quantitative value for the fitting process.  $\chi^2$  is computed by the program as follows. The residual  $r_i$  in each channel (the difference between the sample spectrum and the least-squares spectrum) is computed:  $\sum (y_i - f_i)$ . The variance in channel  $i$  for the least-squares spectrum  $\sigma_i$  is then computed from the formula

$$\sigma_i = (f_i + 0.1) + b_i t / t' (1 + t / t'),$$

Then 
$$\chi^2 = \sum_i r_i / \sigma_i$$

and reduced  $\chi^2$  is 
$$= (1/D_f) \sum_i r_i$$

where  $D_f$  = number of (channels - standards).

### b) "RESULTS + CONCENTRATIONS AND EST STANDARD ERRORS"

The nuclide name, nuclide concentration, and the estimated standard error is printed out for each nuclide, in the "printout" order. The concentration is in the same units as the standards in the nuclide library, and is the "actual" concentration determined by multiplying the "relative" concentration computed by the program multiplied by factors that take into account sample decay, volume reduction and result multiplication, the activity of the standard, and sample and standard counting times. The relative standard error is multiplied by the same factors. Also included in this section of output are the final partial F-values and the corresponding Q- and x-values for each standard in the final set.

### c) "ANALYSIS OF VARIANCE"

This table lists the contributions of the regression and residuals to the total variance. In it are given the degrees of freedom and sums of squares for the regression, residuals and total; the mean sums of square due to the regression and residuals, and the overall F-value. The Mean Square Residual has an expected value for a good fit of  $1.0 \pm (2/D_f)^{1/2}$ .

## (10) "LLNL R-STATISTIC"

This output is the result of the analysis of the residuals from the least-squares fit. It gives the auto-correlation statistic,<sup>7</sup> its expectation value, standard deviation and an approximate associated FAP. A

low value of the auto-correlation coefficient means that the distribution of residuals is random. As this value approaches one (1) the residuals are becoming more correlated, indicating a poorer fit to the data.

#### (11) "FINAL STATISTIC FOR ELIMINATED STANDARDS"

This is a listing of the name and final partial F-value and associated Q- and X-value for each library standard eliminated from the set during the regression. It is useful to determine whether a standard was eliminated because it is truly uncorrelated with the sample or the threshold value for the F-test (variable F0 in UEDIT) was too high.

#### (12) "RATIO OF RESIDUALS OVER STD DEV PER CHANNEL"

The "residual" in each channel is the difference between the sample spectrum and the least-squares spectrum ( $y_i - f_i$ ). The standard deviation for the least-squares spectrum is defined to be

$$\sigma_i = [(f_i + 0.1) + b_i t / t' (1 + t/t')]^{1/2}$$

The program prints out one ratio for each channel in the least-squares spectrum; the printout should be read horizontally from left to right. These ratios, when squared, summed for all channels, and divided by the number of degrees of freedom  $D_f$ , will = "reduced"  $\chi^2$ .

An examination of these ratios reveals where the least-squares spectrum  $f_i$  fits poorly the sample spectrum  $y_i$ , since these ratios will be "large." Ratios  $\geq 10$  or three consecutive ratios  $\geq 2$  are flagged as "suspicious channels" and printed out in the next part of the output.

#### (13) "SUSPICIOUS CHANNELS"

The location and contents of any suspicious channels are given. These are the channels where the ratio of the residual to the standard deviation,  $r_i/\sigma_i$ , is greater than 10 or the central channel of three consecutive channels that are all greater than +2. These are the same ratios that are printed out in the section "Residuals/Standard Deviation per Channel"; the "Suspicious Channels" indicates those channels where the least-squares fit is poor. The "suspicious channels" pointed out may or may not indicate the presence of an unexpected nuclide.

#### (14) "DISTRIBUTION OF RESIDUALS"

This is a histogram plot of the distribution of the residuals/standard deviation per channel. It is preceded by a moment analysis of the distribution of residuals giving the "MEAN," "VARIANCE," "SKEWNESS," and "EXCESS." The shape described by the moments as well as the visual identification of large residuals can be used in determining the "goodness of the fit" to the sample spectrum. In the present version of the subroutine RESID, residuals with  $r_i/\sigma_i \geq 5$  are put in the first or last channel depending on the sign of the residual.

(15) "DISTRIBUTION OF RUNS"

This is a histogram plot of the number of positive and negative runs in the residual spectrum. A run is a series of consecutive channels in the residual spectrum. For a good fit, the expected value for the number of runs, for these spectra, is  $D_f/2 \approx (D_f/4)^{1/2}$ . The presence of large runs or a low number of runs can be an important aid in determining the randomness of the residuals and, hence, the goodness of the fit.

(16) "LOCATIONS AND SIZES OF LARGE RUNS"

The last item in the PREGA output is the location (or starting channel) of the large runs, and the length of the run. The sign of the length denotes whether this is a run of positive or negative residuals. In the present version of the subroutine RUNS only runs of absolute length five or greater are output.

VARIABLES (PREGA)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
A(10,10)	Square matrix to be inverted
AC(10)	Activity of standards from library
ARR(10,64)	Matrix containing 64 channels of (max.) 10 standard spectra; for residual calculation
ASC(60)	Disk locations of standard spectra
B(10)	$C_j = \sum_i w_i a_{ij} x_i$
BA(512)	Spectrum for either standard background or sample background, depending on location in program
BR	User option to do regression with trial set consisting of; = 0 all standards chosen = 1 background only
	NOTE: FOR BR=1; BACKGROUND MUST BE STANDARD No. 1 IN THE LIST
C	Bit pattern of standards currently in regression for present pivot
CC(10,10)	Correlation matrix for standards and sample
CH	$x^2$ value for least-square spectrum
CHDF	= CH/DN; "reduced" $x^2$ for least-squares spectrum

# VARIABLES (PREGA) (Cont'd)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
D	Bit pattern of standards removed from original set
DAY	Decay time of sample (seconds)
DEF(10)	Hollerith constant DEF 8,
DF	Degrees of freedom; $NCH-P$
DG	Regression degrees of freedom; N
DN	Degrees of freedom; the number of channels used in the least-squares fit minus the number of standard isotopes
DR	Residual degrees of freedom; $MF-NZ-P+1$
DT	Total degrees of freedom; $DG+DR$
E	Bit pattern integer for standards currently in regression analysis
EF(10)	Logical variable to keep track of standard status in subroutine PIVOT
F	Bit pattern integer of original set of standard nuclei used
F $\phi$	F-test rejection coefficient
FAT	$t/t'$ ; counting time of standard divided by counting time of standard background
FD	Correction for decay of sample and standard
FF	Final F-statistic = $XG/XR$
FILE	Logical unit number 8 (disk file:spectra)
FMAX	Maximum F-value (I) in forward pivot
FMIN	Minimum F-value (I) in backward pivot
FP(10)	F-value (I) after doing pivot
FPM(10)	F-value (I) for "F-to-remove" or "F-to-add"
FPS	Partial F-value sent to subroutine XQCALC
FS	$t/t'$ ; counting time of sample divided by counting time of sample background

VARIABLES (PREGA) (Cont'd)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
FX	$t/t'(1 + t/t')$ ; second order correction term for time difference
HA(10)	Half-life of standards from library: input library order
HAT(10)	Half-life of standards; printout order
HF(5)	Hollerith output variable for titles
HG	Hollerith output variable for titles
HH(6)	Hollerith output variable for titles
HR	Hollerith output variable for titles
HT	Hollerith output variable for titles
I	Index used for nuclide and channel number
I <sub>0</sub>	Beginning of loop over standards value
I <sub>1</sub>	End of loop over standards value
IDAT	Associated variable for logical units 9 and 11
IFORKL(30)	Variable format statement number associated with ENCODE statement
IFORN(20)	Variable format statement number associated with ENCODE statement
II	Index used in library standards read/write operations
IN	Integer resulting from checking if standard I is in the current list before a pivot
INEG	Integer used to check sign of partial correlation coefficient ( $R2=RHO*RHO$ )
IPO	Integer used to direct program in next step after output of a pivot result
IR(512)	Suspicious channel number
IS(10)	Printout order of standards; OR in UEDIT can change as program is executed

VARIABLES (PREGA) (Cont'd)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
ISL(10)	Printout order of standards; OR in UEDIT never changes during execution
IT(10)	Serial order of standards to be used in least-squares fit
IVAR	Associated variable for logical units 8 and 10
J	Index used for nuclide and channel number
JJ	Index used with ASC for sample and background spectra
JJJ	Do loop counter
JDF	Standard set F minus standard set D, used at end of backward pivot
K	Index used for nuclide and channel number
KAC	Variable associated with ENCODE statement for format 916
KRO	Output residual (Yes = 1, No = 0)
LN	Number of standards used plus 1, $N + 1$
LOOP	Integer to read 64 channels from disk for residual calculation
LSK	Variable associated with ENCODE statement for format 916
LW	User option for weighting factor $p_i$ ; WF in UEDIT if based on actual counts $= 1$ for $p_i = 1$ $= 0$ for $p_i = 1/(\text{sample counts} + \text{background counts})$ $= -1$ for $p_i = 1/(\text{sample counts} + 1.0)$
M	Number of channels of standard and sample spectra (max = 512)
MF	Final channel number for computation
MI	Logical unit 9 (disk file: nuclide library)
MIU	Logical unit 11 (disk file: unknown sample)
MO	Logical unit 6 (line printer)

# VARIABLES (PREGA) (Cont'd)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
MP	= 6 logical unit number of line printer
MY(10)	Integer vector used to check bit pattern of current set of standards for a particular standard
N	Number of standard nuclides to be fit (max = 9)
N2	Maximum channel number minus two; used for suspicious channels calculation
N5	Used to represent one (specified by program) value from IS or IT array
N6	Used to represent one (specified by program) value from IS or IT array
NBA	User option for standard background subtraction; BS in UEDIT = 1 for subtraction = 0 for no subtraction
NBR	User option for background; BG in UEDIT = 1 for background supplied = 0 for no background supplied
NBS	User option for sample background subtraction = 1 subtraction = 0 no subtraction
NCH	Number of channels used for calculation; MF-NZ+1
NDET	= 0 dead time correction (0 = no, 1 = yes)
NEWST	User option for application of rejection coefficient; RC in UEDIT = 1 for application = 0 for no application
NIT	Carry over from old NAI program. To be eliminated when SEDIT and UEDIT are restructured
NNN	= 0 counter index used in calling subroutine DECAY
NS	Number of standard spectra in library (maximum = 40)
NW	User option for weighting factor p <sub>i</sub> ; WD in UEDIT

# VARIABLES (PREGA) (Cont'd)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
NZ	Initial channel used for calculation
P	Number of standards currently in regression
Q	Rejection coefficient; RC in SEDIT
QF	Q(X) associated with F-values
QH	User defined threshold channel number, TC in UEDIT
R(512)	1. Standard spectra (up to line 493) then 2. Ratio of residual divided by standard deviation
R2	Concentration of standard squared divided by standard error of standard divided by residual sum of squares; used to calculate partial F-values for PIVOT; partial correlation coefficient
RE	Residual count; $RE = Y(J) - SV$
RHO	Square root of partial correlation coefficient, R2
RMSR	Residual sum of squares divided by Df
RSS	Residual sum of squares
RT	$x^2$ sum for least-squares spectrum
S(512)	Standard spectra counts; $a_{ij}$
S1	$= \sum_i x_i$ ; sum of counts for the sample spectrum
S2	$S1 + SB * FX$ ; sum of sample plus corrected background counts
SA	$b_{jk}$ ; least square sum coefficients for unknown concentrations $Z(I)$ and sample $Y(I)$ ; store in $A(L,K)$ ; total sum of squares
SB	Sum of counts for the sample background spectrum from the initial to the final channel
SG	Regression sum of squares
SIR(50)	Contents of suspicious channels
SNAM(2)	Sample file name used in output for identification

# VARIABLES (PREGA) (Cont'd)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
SQUC	Used to check sign of number before taking square root
SR	Residual sum of squares
SRD1	$\sigma_{II}$ for correlation coefficient CC(I,J)
SRD2	$\sigma_{JJ}$ for correlation coefficient CC(I,J)
SS(10)	$\sum_i a_{ij}t_j$ ; sum of counts for standard isotopes from the initial to final channel
ST	Residual sum of squares
STD(10)	1. Variance of the nuclide concentration; input library order 2. Corrected standard error of the nuclide concentration; input library order
SUM	Relative nuclide concentration, $m_j$
SUM W	Sum of weighting factors, $P_i$ , from initial channel to final channel
SV	Least squares spectrum sum, $\sum_i f_i$
SX	$c_j$ , least squares sums for constant terms
T	1. $Y(I)*BA(I)*FX$ defined at program line 2. Reciprocal of $p_i$ defined at program line 3. $r^2$ ; residual squared defined at program line 480
TB	Counting time for background
TE	1. $Y(J)*BA(J)*FX$ used in calculation of CHDFS
TIS1	Hollerith constant to store "SAMP"
TIS2	Hollerith constant to store "LE "
TISO(20)	Names of stored nuclides used in least squares fit; in printout order
TISOT(40)	standard nuclide names; input library order
TMO	$= (0.1 + SV)$ ; reciprocal of $p_i$ based upon least-squares spectrum

## VARIABLES (PREGA) (Cont'd)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
TMP	= TMO + BA(J)*FX; reciprocal of $p_j$ based upon least-squares spectrum + corrected background; defined at program line 484. Redefined at program line 493 as the square root of TMP.
TNAME(36)	Original location of sample spectrum
TSA	Counting time for sample in seconds
TST(10)	Counting time of standard in seconds; from PREGA library
VM	User defined result multiplication factor; MF in UEDIT
VRED	User defined volume reduction factor; VR in UEDIT
VU	Sum of residuals squared
VVV	Sum of TMP
VY	Residual squared times $p_j$
W(512)	Weighting factors $p_j$
XF	X-value returned from subroutine XQCALC and checked against $F_0$
XG	Final regression sum of squares divided by degrees of freedom
XR	Final residual sum of squares divided by degrees of freedom
Y(513)	Sample spectrum $X_j$
Z(10)	Library nuclide concentration
ZS	Nuclide concentration sent to subroutine XQCALC

### Program Calculations

PREGA is a FORTRAN language program consisting of approximately 638 lines and requiring ~ 52K words of memory for execution. The main calculation steps used by the program to calculate the best subset of standards using the pivotal regression technique, the nuclide concentration, residuals and the statistical analysis of accidental errors are listed on the following pages. This section is included to provide further understanding of the calculation and as a guide for future modifications that may become necessary or desirable.

# PREGA Program Calculations

Program Line Number	FORTTRAN Expression	Description	Equation Number
70	FAT = TST(I)/TB	Counting time of standard i counting time of background	1
72	S(J) = S(J)-BA(J)*FAT	[Standard counts - corrected background counts] in each channel summed over all channels	2
103	FS = TSA/TB	Counting time of sample counting time of background	4
104	FX = FS + FS**2	Second order correction factor used in line 484	5
121	Y(I) = Y(I)-BA(I)*FS	[Sample counts - corrected background counts] in each channel i	6
124	SB = SB + BA(I)	Total background counts; this is the "BACKGD SUM" that is printed out	7
129	S1 = S1 + Y(I)	Total sample counts (corrected background subtracted); this is the "SAMPLE SUM" that is printed out	8
211	SS(L) = SS(L)+R(J)/W(J)	Weighted sum of standard counts in all channels i for nuclide j; this is the "WEIGHTED SUM OF STANDARDS AND UNKNOWN" that is printed out	3

\*\*\*SET UP ARRAY A(N+1, N+1) AND CORRELATION MATRIX\*\*\*

# PREGA Program Calculations (Cont'd)

Program Line Number	FORTRAN Expression	Description	Equation Number
216	S(J) redefined as original standard spectra	FORTRAN S(J) here represents the standard spectra	
219	SA=SA+S(I)*R(I)*W(I)	Standards cross product terms times weighting factor stored in A(L,K)	9
225	SA=SA+R(I)*Y(I)*W(I)	Cross product of standards and sample terms stored in A(N+1,L) and B(L)	10
233	SA=SA+Y(I)*Y(I)*W(I)	Stored in A(N+1, N+1); this location is the residual sum of squares during the pivot operations. Also stored in ST	11
244	SRD1=A(K,K)-SS(N6)**2/SUMW	Variance of standard K (or sample)	12
245	SRD2=A(L,L)-SS(N5)**2/SUMW	Variance of standard L (or sample)	13
246	CC(K,L)=(A(K,L)-SS(N6)*SS(N5)/SUMW) /SQRT(SRD1*SRD2)	Correlation coefficient: covariance of standards K and L divided by the square root of the product of their variances	14
***START PIVOTAL REGRESSION ANALYSIS***			
329	FPM(I)=(NCH-P)*((A(I,LN)**2)/ (-A(I,I)*A(LN,LN)))	Calculate partial F to remove; NCH-P = degrees of freedom	15

# PREGA Program Calculations (Cont'd)

Program Line Number	FORTTRAN Expression	Description	Equation Number
381	FPM(I) = ((NCH-P-1)*R2)/(1.0-R2)	Calculate pal F to add; NCH-P-1 =degrees of freedom	16
409	RSS = A(LN, LN)	Residual sum of squares	
410	RMSR = RSS/DF	Residual sum of squares per degree of freedom	
418	Z(J) = -A(I, LN)*TST(N5)/TSA	Relative concentration of standard J	17
422	STD(J) = SQRT(SQUC)*RMSR *TST(N5)/TSA	Relative standard error of standard J determined from the variance	18
448	SG=SG-A(I, LN)*B(I)	Regression sum of squares	
475	SV = SV+ARR(JJ, JJJ)*(-A(I, LN))	Calculates the least-squares spectrum counts in each channel (because of memory limitations, this is done 64 channels at a time)	19
479	RE = Y(J)-SV	Residual = difference between sample and least-squares spectrum	20
480	T = RE**2	Squares the residual	21
481	VY = VY+W(J)*T	Residual sum of squares; stored in SR at line 472	22
482	VU = VU + T	Sum of residuals squared over all channels	23
483	TMO = ABS(0.1 + SV)	f <sub>1</sub> must ≠ 0; zero divide prevention	24

' PREGA Program Calculations (Cont'd)

Program Line Number	FORTRAN Expression	Description	Equation Number
484	TMP = TMO + BA(J)*FX		25
485	VVV = VVV + TMP	Accumulates TMP over all channels	26
491	RT = T/TMP	Residual squared TMP	
492	CH = CH + RT	Accumulates RT over all channels; this is chi-squared for least-squares spectrum	27
493	TMP = SQRT(TMP)	Redefine TMP as square root of TMP	
494	R(J) = RE/TMP	Calculates residuals over standard deviations; printed out as "RATIO OF RESIDUALS OVER STD DEVIATION PER CHANNEL"	
498	DN = MF-P-NZ+1	Calculates the number of degrees of freedom for $\chi^2$ , MF = end channel, NZ = start channel, P = number of standards in fit	
501	DT = DR+DG	Total number degrees of freedom	
502	CHDF = CH/DN	"Reduced" $\chi^2$ for the least-squares spectrum; this is the "FIT" that is printed out	
513	FD = EXP(0.693*DAY/HA(N5))	Correction for decay of sample DAY = $t_{1/2}$ =half-life of sample and HA = $T_{1/2}$ =half-life of standard	28
514	STD(J)=SQRT(-A(I,I)*A(LN,LN)/DN) *TST(N5)/TSA	Relative standard error determined from variance of standard 1	

# PREGA Program Calculations (Cont'd)

Program Line Number	FORTTRAN Expression	Description	Equation Number
515	STU(J)=AC(N5)*FD*STD(J)*VM/VRED	Corrected standard error; AC is the activity of the sample; VM is result multiplication factor; VRED is volume reduction factor	
516	Z(J)=(-A(I,LN))*(TST(N5)/TSA)*AC(N5)*FD*VM/VRED	Relative concentration $m_j$ is converted to actual concentration level	
526	XG = SG/DG	Reduced regression sum of squares	
527	XR = SR/DR	Reduced residual sum of squares	
528	FF = XG/XR	Final F-statistic	

Equations Used in PREGA (FORTRAN variables are underlined)

1.  $\underline{FAT} = t_j/t'$
2.  $\underline{S(J)} = \sum a_{ij} = \sum S_{ij} - b_i(t_j/t')$
3.  $\underline{SS(J)} = \sum a_{ij}$
4.  $\underline{FS} = t_s/t'$
5.  $\underline{FX} = (t_s/t')(1 + t_s/t')$
6.  $\underline{Y(I)} = x_i = z_i - b_i(t_s/t')$
7.  $\underline{SB} = \sum b_i$
8.  $\underline{S1} = \sum x_i$
9.  $\underline{A(L,K)} = \sum a_{ik}a_{il}w_i$
10.  $\underline{SA} = \sum a_{il}x_iw_i$
11.  $\underline{SA} = \sum x_ix_iw_i$
12.  $\underline{SRD1} = \sigma_{kk} = A_{kk} - (\sum a_{ik}w_i)^2 / \sum w_i$
13.  $\underline{SRD2} = \sigma_{ll} = A_{ll} - (\sum a_{il}w_i)^2 / \sum w_i$
14.  $\rho_{kl} = \frac{A_{kl} - \left[ \sum_i a_{ik}w_i \sum_i a_{il}w_i / \sum_i w_i \right]}{(\sigma_{kk} \sigma_{ll})^{1/2}}$
15.  $F_p^- = DF * R^2 = DF * A_{I,N+1}^2 / (-A_{II} A_{N+1,N+1})$

Equations Used in PREGA (FORTRAN variables are underlined) (Cont'd)

$$16. \quad F_p^+ = DF \cdot R^2 / (1-R)^2$$

$$17. \quad \underline{Z(J)} = \sum_i a_{ij} \cdot t_j / t' = m_j$$

$$18. \quad \underline{STD(J)} = (A - (I, I) \cdot A(N+1, N+1) / DF) t_j / t'$$

$$19. \quad \underline{SV} = f_i = \sum_j a_{ij} m_j$$

$$20. \quad r_i = (x_i - f_i)$$

$$21. \quad r_i^2 = (x_i - f_i)^2$$

$$22. \quad \underline{VY} = \sum_i r_i^2 w_i$$

$$23. \quad \underline{VU} = \sum_i r_i^2$$

$$24. \quad \underline{TMO} = 0.1 + f_i$$

$$25. \quad \underline{TMP} = (0.1 + f_i) + b_i \underline{FX}$$

$$26. \quad \underline{VVV} = \sum (0.1 + f_i) + b_i \underline{FX}$$

$$27. \quad \underline{CH} = \sum r_i^2 / (0.1 + f_i) + b_i \underline{FX}$$

$$28. \quad \underline{FD} = \exp(0.693 \cdot t_{1/2} / t_{1/2}^S)$$

## Software Organization

### (1) Logical Unit and Disk File Structure

The program PREGA and the two editor programs SEDIT and UEDIT have access to data stored in disk files via specific, user-defined logical units. The organization of these programs, disk files, and logical units is shown in figure 2.

The program PREGA uses logical units 6, 8, 9, 10, and 11. It shares logical unit 9 with the SEDIT editor program and shares logical unit 11 with the UEDIT editor program.

Logical unit 6 is used to print out the results of the program; it is usually a line printer.

Logical unit 8 is a disk file that stores spectral data that have been accumulated by the user in the laboratory. The program PREGA reads this data to perform its calculations. Each spectrum is stored in one disk file element. The data will include the sample spectrum, the background spectrum for the sample, the standard spectra (up to 9 standards are permitted at present) and the background spectrum for the standard. The background spectrum must be standard No. 1 in the library.

Logical unit 9 is the standard nuclide library file. The file contains information common to all nuclides in the library (the file "header") as well as specific information about each nuclide (the "list of standards"). For each standard spectrum in logical unit 8 there will be a corresponding entry in the nuclide library file. The editor program SEDIT is used to add, delete, or make changes in this file.

Logical unit 10 is used by the program PREGA for temporary storage of large data arrays. This is a "scratch" file.

Logical unit 11 is a disk file that contains information about the unknown spectrum the user has acquired. The UEDIT editor program is used to add, delete or change the information in this file.

The file structures for logical units 8, 9, 10, and 11 are shown on the following pages. The file structures for logical units 9 and 11 show two columns of program parameter names. The editor programs use the names in the first column and the program PREGA uses the names in the second column.

The following relation exists among sectors, records, words, bytes, and bits for all files defined as logical units 8, 9, 10, and 11 in the program PREGA:

1 sector = 64 records = 128 words = 256 bytes  
1 record = 2 words = 4 bytes = 32 bits  
1 word = 2 bytes  
1 byte = 8 bits

(1a) Logical Unit 8

The program PREGA uses the GET subroutine to read each spectrum through logical unit 8. Each file element contains one spectrum. The spectral data begins with record number 129 (decimal byte offset 512); the first 128 records (511 bytes) in each file element are not used by PREGA. The first 128 records comprise the Header section of Nuclear Data spectral files and contain information used by other programs (e.g. GSHIFT, GET, PUT).

The numbering system is illustrated below for the first 2 records.

Word 2	Word 1	Record 129
byte 515   byte 514	byte 513   byte 512	
Word 2	Word 1	Record 130
byte 519   byte 518	byte 517   byte 516	

Data type coding is as follows:

Sptr (Spectral data) The spectral data from each channel is stored in 4 bytes. Only 30 bits are used. The values are stored as double integers. Word 1 is the least significant word.

Regardless of the number of bits/channel assigned to an ADC, each channel is always written to disk as a 32-bit word.

If  $M$  = the number of channels of spectral data, the decimal byte length of the file element is  $512 + 4 * M$ . The user can use this to determine how much disk space must be reserved for the spectral data. For example, the maximum number of channels a user can have in one spectrum is 512. This would require 2560 bytes or 10 sectors to be reserved for that file element. The maximum number of spectra accessible by SEDIT at any given time is currently 9. The number of spectra which can be stored on the disk in file DATA is determined by the size of file DATA. Because SEDIT is limited to 9 standards, the maximum number of spectra, or file elements a user can have on logical unit 8 is 12 (see below) so the upper limit of the size of this disk file is 120 sectors.

The total number of file elements will be the sum of:

- 1 to 9 file elements for the standard spectra
- 1 file element for the standard background spectrum
- 1 file element for the unknown sample spectrum
- 1 file element for the unknown sample background spectrum

NOTE - The program SEDIT can actually handle up to 40 standard spectra. The limitation of only 9 standard spectra is caused by PREGA. As stated earlier, PREGA was built on the framework of the Nuclear Data, Inc. NAI analysis program, which has some built-in inefficiency. The method for modifying PREGA and, hence the whole package is given in more detail below. At present, it was felt that 9 standards would be sufficient for the present analysis without making PREGA unnecessarily larger.

# Structure of PREGA File 8

<u>Record Number</u>	<u>Decimal Byte Offset</u>	<u>Decimal Byte Length</u>	<u>Parameter Description</u>	<u>Data Type</u>
1	0	4	Not used	...
2	4	4	Not used	...
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
128	508	4	Not used	...
129	512	4	Number of counts in channel 1	Sptr
130	516	4	Number of counts in channel 2	Sptr
131	520	4	Number of counts in channel 3	Sptr
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
641	2560	4	Number of counts in channel 512	Sptr

(1b) Logical Unit 9

SEDIT writes the file to logical unit 9 and the program PREGA reads from logical unit 9.

The numbering system is illustrated below for the first 2 records.

Word 2	Word 1	Record 1
byte 3    byte 2	byte 1    byte 0	
Word 2	Word 1	Record 2
byte 7    byte 6	byte 5    byte 4	

Data type coding is as follows:

- A    ASCII characters
- F    REAL\*4 single precision floating point with 4 bytes
- I\*2   INTEGER\*2 with 2 bytes
- L\*1   LOGICAL\*1 with 1 byte

The number in the "offset" column is the address.

This file requires 256 bytes for the "header" section and 64 bytes for each nuclide in the library. If N represents the number of nuclides in the library, then a total of  $256 + 64N$  bytes of storage are required; one sector = 256 bytes. For example, the maximum number of nuclides a user can have in the library is 9. This would require  $256 + 576 = 832$  bytes. An example printout of this file is given in the section about SEDIT. The example consists of two parts: the first part is the "PREGA LIBRARY HEADER" and the second part is the "PREGA LIBRARY STANDARDS".

# Structure of PREGA and SEDIT File 9

<u>Record Number Offset</u>	<u>Decimal Byte Offset</u>	<u>Decimal Byte Length</u>	<u>SEDI T Name</u>	<u>PREGA Name</u>	<u>Parameter Description</u>	<u>DATA Type</u>
1	0	2	M	NS	number of isotopes in standard library (max = 9)	I*2
2	4	2	NC	M	number of channels per standard (max = 512)	I*2
3	8	2	IT	NIT	number of iterations for threshold and gain calculation (not used)	I*2
4	12	2	BS	NBA	background subtract 1 = yes, $\phi$ = no	I*2
5	16	2	IS	NZ	initial channel for computation	I*2
6	20	2	IE	MF	final channel for computation	I*2
7	24	132			space reserved for file expansion	
40	156	4	BT	TB	counting time for standard background	F
41	160	4	RC	Q	rejection coefficient	F
42	164	30	BA	ASC	standard background location	L*1
49	194	2			word 2 of record 49 not used	
50	196	60			space reserved for file expansion	
65	256	8	A	TISOT	first standard isotope name	A
67	264	30	A	ASC	first isotope location	L*1
74	294	2			word 2 of record 74 not used	
75	296	4	HL	HA	half-life of first isotope	F
76	300	4	SEC	TST	counting time of first isotope	F
77	304	4	ACT	AC	activity of first isotope	F
78	308	12			not used	
81	320	52			data for standard isotope two	
94	372	12			not used	
97	384	52			data for standard isotope three	
110	436	12			not used	

.

.

.

through 65+ (NS\*16) -3

where NS = number of isotopes in standard library

The second word of records 1,2,3,4,5 and 6 is not used.

(1c) Logical Unit 10

PREGA reads and writes to the file of the logical unit 10. This file, a "scratch" file, is used for temporary storage of the large data arrays manipulated by the NAI program.

The numbering system is illustrated below for the first 2 records.

Word 2	Word 1	Record 1
byte 3    byte 2	byte 1    byte 0	
Word 2	Word 1	Record 2
byte 7    byte 6	byte 5    byte 4	

Data type coding is as follows:

Sptr (Spectral Data) The spectral data from each channel is stored in 4 bytes. Only 30 bits are used. The values are stored as double integers. Bits 14 and 15 have been set for 0 for word 2, which is the most significant word.

Structure of PREGA File 10 ("Scratch" file)

<u>Record Number Offset</u>	<u>Decimal Byte Offset</u>	<u>Decimal Byte Length</u>	<u>PREGA Name</u>	<u>Parameter Description</u>	<u>DATA Type</u>
1	0	4*M	S	storage for all channels of first standard spectrum	Sptr
M+1	4*M	4*M	S	storage for all channels of second standard spectrum	Sptr
2*M+1	2*4*M	4*M	S	storage for all channels of third standard spectrum	Sptr
3*M+1	3*4*M	4*M	S	storage for all channels of fourth standard spectrum	Sptr
.	.	.	.	.	
.	.	.	.	.	
.	.	.	.	.	
NS*M+1	NS*4*M	4*M	S	storage for all channels of sample spectrum	Sptr

where M = number of channels per standard

NS = number of isotopes in standard library

(1d) Logical Unit 11

UEDIT writes the file to logical unit 11 and PREGA reads from logical unit 11.

The numbering system is illustrated for the first 2 records.

Word 2	Word 1	Record 1
byte 3    byte 2	byte 1    byte 0	
Word 2	Word 1	Record 2
byte 7    byte 6	byte 5    byte 4	

Data type coding is as follows:

F    REAL\*4 single precision floating point with 4 bytes

I\*2 INTEGER\*2 with 2 bytes

L\*1 LOGICAL\*1 with 1 byte

The number in the "offset" column is the address.

An example of the printout of this file is given in the section on UEDIT with the heading "PREGA UNKNOWN SAMPLE PARAMETERS".

# Structure of PREGA and UEDIT File 11

Record Number	Decimal Byte Offset	Decimal Byte Length	UEDIT Name	PREGA Name	Parameter Description	DATA Type
1	0	4			dummy	
2-9	1	30	UN	ASC	location of sample spectrum	L*1
9	34	2			word 2 of record 9 not used	
10	36	4	GN	FIT	gain shift ratio (not used)	F
11	40	4	TH	SHCT	threshold shift (not used)	F
12	44	2	BG	NBR	background supplied yes = 1 no = 0	I*2
13	48	2	BS	NBS	background subtract yes = 1, no = 0	I*2
14	52	4	BT	TB	counting time for sample background (sec)	F
15	56	4	CT	TSA	counting time for sample (sec)	F
16	60	4	VR	VRED	sample concentration factor	F
17	64	4	DT	DAY	decay time (sec)	F
18	68	4	MF	VM	sample dilution factor	F
19	72	30	BA	ASC	location of sample background	L*1
27	104	2			word 2 of record 27 not used	
28	108	2	WD	NW	weighting factor determination: = 0 if based on actual counts/channel = 1 if based on calculated counts/channel	I*2
29	112	2	NS	N	number of library spectra to be fitted to the sample	I*2
30	116	2	F0	F0	F-test rejection coefficient	R*4
31	120	2	WF	LW	weighting factor = -1 for (sample counts +1) **-1 = 0 for (sample counts + back- ground counts)**-1 = 1 for 1	I*2
32	124	2	RC	NEWST	apply rejection coefficient	I*2
33	128	2	BR	BR	start regression with background only; 0 = no, 1 = yes	I*2
34	132	2	BP	BP	allow pivot on background 0 = no, 1 = yes	I*2
35	136	2	RO	KRO	output residuals 0 = no, 1 = yes	I*2
36	140	32	RS	ASC	ID of output file for residuals	L*1
43	176	4*N	OR	IS	library standard number listed in the order of desired printout	I*2

N is the number of library nuclides to be fit to the sample.

The second word of records 12,13,27,28,29,30,32,33,34, and 35 through 43+N is not used.

## Subroutines Called by the Program PREGA

The following eleven subroutines are used during the execution of PREGA. Figure 3 shows the hierarchy of subroutine calls. Brief descriptions of each subroutine are given below. Listings of the subroutines are given in Appendix B.

### (1) GET+(ASC, ARRAY, IVAR, FILE, M)

The subroutine GET is used by the NAI program to obtain spectral data from the various disk file/elements defined as logical unit 8. The program PREGA first obtains the location of the spectrum and sends this location, as an ASCII character string, to the GET subroutine. GET in turn calls CONCAT which concatenates the character string and LUNDEF subsequently sends the concatenated string to the operating system, MIDAS, which interprets the string and performs the command operation. GET is a FORTRAN language subroutine, while the other two, CONCAT and LUNDEF, are written in assembler language.

Listings or descriptions of the system routines CONCAT and LUNDEF are given in Appendix C.

### VARIABLES (GET)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
ARRAY(256)	Channel Contents of Spectrum Being Retrieved from Disk
ASC(60)	Location of spectrum being retrieved (FILE. ELEMENT (, DEVICE))
DEF(10)	Hollerith constant DEF8, used to create a command in CONCAT and LUNDEF
FILE	Logical unit number 8 (disk file:spectra)
IVAR	Associated variable for logical unit 8
K	Loop index over number of channels in spectrum
LSB	Least significant byte of data word
M	Number of channels in spectrum
MSB	Most significant byte of data word
NAM(60)	Concatenated character string ASC sent to LUNDEF
RE1	Most significant byte of data word ARRAY(K) converted to R*4
RE2	Least significant byte of data word ARRAY(K) converted to R*4

(2) HISTO (LABEL, IH, XL, XD, N)

The FORTRAN subroutine HISTO is called by the Subroutines RESID and RUNS. From the data received from these two subroutines it generates a labeled, scaled histogram which is output to logical unit 6. The two histograms are "DISTRIBUTION OF RESIDUALS" and "DISTRIBUTION OF RUNS". This routine was written by G. Phillips at NRL in June of 1981.

VARIABLES (HISTO)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
A(50)	Data point character '*'
ASTAR	Data point character '*'
ACOLON	Data point character ':'
I	Loop index to skip 5 lines after histogram is output
IDIV	Scale factor for output histogram
IH(21)	Number of steps on x-axis (21 MAX)
IOUT	Logical unit = 6 for output
IT	$\sum x_i$ for output histogram
J	Y-value for each channel x
K	Loop over number of x-values in histogram
LABEL (4)	Title label for output histogram
MAX	Maximum Y-value allowed; used to determine scale factor (MAX/IDIV $\leq$ 50)
N	Number of x-values in histogram
X	First (or lowest) x-value
XD	Step size of x-values
XL	Lowest x-value from calling program

### (3) PIVOT (A,P,E,K)

PIVOT is a FORTRAN subroutine called by PREGA. Its purpose is to produce the negative of the upper triangle of the inverse of a square symmetric matrix by operating only on the upper triangle of the matrix. The procedure by which this is accomplished is an adaptation of the Gauss-Jordon Method. On each entry to PIVOT a specified diagonal element is used for one pivot operation. To invert a  $k^{\text{th}}$  order matrix the procedure must be called  $k$  times. The order of which diagonal element is pivoted is unimportant. This routine checks for a near-zero pivot. All pivots are done with single-precision arithmetic with no significant loss of accuracy. The routine was written in FORTRAN by G. Phillips and B.G. Glagola, NRL in July 1982 from Algorithm AS 37 by M.J. Garside.<sup>3</sup>

#### VARIABLES (PIVOT)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
A(10,10)	Array of standards and sample to be inverted
AA	Reciprocal of the element about which the pivot occurs (A(P,P))
AIP	A(I,P)*AA or A(P,I)*AA
E(10)	Variable to determine which standards are in the current subset
I	Loop index over standards with array index less than that of the pivoting standard (max P1 = P-1)
J	Loop index over standards and sample with array index greater than that of the pivoting standard (min P2 = P+1)
K	Number of standards in original set plus one (in PREGA K = LN = N+1)
P	Index of the pivoting standard
P1	P1 = P-1; loop maximum
P2	P2 = P+1; loop minimum

(4) PUT (ASC, ARRAY, IVAR, FILE, M)

The FORTRAN subroutine PUT was written by G. Phillips, NRL in June 1981. PREGA uses PUT to write the residual spectrum on disk using logical unit 8. This routine also uses CONCAT and LUNDEF to send a character string to the MIDAS operating system and perform the command.

VARIABLES (PUT)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
ARRAY (256)	Spectrum to be output to disk
ASC (60)	Disk location of spectrum (File. Name (, Device))
DEF (10)	Hollerith constant DEF 8, used to create a command in CONCAT and LUNDEF
FILE	Logical unit number 8
IVAR	Associated variable for logical unit 8
K	Loop index over number of channels in output spectrum
LSB	Least significant byte of data word ARRAY(K)
M	Number of channels in output spectrum
MSB	Most significant byte of data word ARRAY(K)
NAM	Concatenated character string ASC sent to LUNDEF
V	Data word ARRAY(K)

(5) RESID (R, NZ, MF)

The FORTRAN subroutine RESID was written by G. Phillips, NRL in June 1981. It is used by PREGA to generate a distribution of residuals from the residual/standard deviation spectrum and perform a moment analysis of this distribution. The output from RESID is the "MEAN RESIDUAL", "VARIANCE", "SKEWNESS", and "EXCESS" of the distribution. RESID also calls HISTO to generate and output the histogram of the distribution of residuals.

## VARIABLES (RESID)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
A(10)	Moments of the residual distribution
C(10)	Constants for the moment calculations
EX	Excess of the residual distribution
I	Index for loop over the number of channels in the residual spectrum
IH(21)	Number of steps on the x-axis for SUBROUTINE HISTO
IOUT	Logical unit for output = 6
J	Index for the loop to calculate $C_j$
K	Index for yield at each step on x-axis for HISTO
LABEL (4)	Title for histogram sent to HISTO
M	Number of channels used in calculation plus 1
MF	Initial channel used in calculations
N	Number of data points sent to HISTO
NZ	Final channel used in calculations
R(256)	Residual/standard error spectrum
SD	Second moment of residual distribution
SQ	Third moment of residual distribution, skewness
U	Mean residual
U2	Mean squared residual
U3	Mean cubed residual
U4	Mean fourth power residual
V	Variance of residual distribution
XD	Step size for HISTO
XL	Lowest x-value for HISTO

(7) RSTAT (NCH, P, R, NZ, MF)

The subroutine RSTAT analyzes the residual/standard deviation spectrum from PREGA to compute an auto-correlation coefficient, its expectation value, standard deviation and an approximate associated FAP. RSTAT uses an entry to the subroutine XQCALC to calculate the associated FAP. This version of RSTAT is an adaptation to PREGA by B.G. Glagola, NRL, 20 July 1982 of the original routine written by T.B. Gosnell, LLNL, 22 June 1982.

VARIABLES (RSTAT)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
CH	Number of channels in residual spectrum
DF	Number of degrees of freedom
EP	Number of standards in final set
EXRES	Expectation value of residual auto correlation coefficient
I	Index for loop over number of channels minus one
MF	Final channel in spectrum
MF1	MF-1
NCH	Number of channels in spectrum from PREGA
NRMR	Equivalent normal standard deviations
NZ	Initial channel in spectrum
P	Number of standards in final set from PREGA
Q	Residual statistic "False Alarm Probability" returned from XQCALC
R(512)	Residual/standard error spectrum from PREGA
RSTT	Auto-correlation coefficient
SIGRES	Standard deviation of R-statistic

(8) RUNS (R, NZ, MF)

The FORTRAN subroutine RUNS analyzes the residual/standard deviation spectrum from PREGA for runs of consecutive channels with the same sign. It outputs the location (starting channel of a run) and the size of the run. The sign of the size indicates a run of positive or negative residuals. RUNS also calls HISTO to generate and output a histogram of the distribution of runs. This routine was written by G. Phillips, NRL, June, 1981.

VARIABLES (RUNS)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
I	Index used for channel counting
ICH	Beginning channel of a particular run
IH(21)	Counter for the number of times a particular run length occurs
J	Output index over location and number of large runs
K	Index for x-axis of number of runs histogram
KSI(12)	Storage variable for length of long runs
LABEL(4)	Identification label for histogram, sent to HISTO
MF	Last channel of spectrum used for calculations
N	Number of data points sent to HISTO
NCH(50)	Initial channel of long runs for output
NRS(50)	Length of long runs for output
NZ	Initial channel of spectrum used for calculation
R(256)	Residual/standard error spectrum from PREGA
XD	Step-size of x-axis of output histogram
XL	Lowest value on x-axis of output histogram

### Future Modifications of PREGA

The program SEDIT, as received originally from Nuclear Data, Inc., is capable of handling up to 40 standard nuclides in the library. At the present PREGA limits the number of standards that are allowed to be in the library. This is because PREGA was built on the framework of the Nuclear Data, Inc. NAI Analysis Package. In this package, the analysis program (called PREGA now) reads control parameters first from SEDIT and then from UEDIT. Hence, PREGA reads all of the standards listed by SEDIT from disk, and computes their sums and does background corrections before it reads from UEDIT which standards and in which order they are to be used in the regression analysis. To keep PREGA from becoming unnecessarily large, it was decided that nine standards would be sufficient to fit a sample spectrum. To increase the maximum number of standards allowed several variable dimensions in PREGA and subroutine PIVOT have to be modified. Currently these have the dimension (10) or (10,10) for arrays. These variables are listed below along with their identification, with N = maximum number of standards in the library.

#### PREGA

A(N+1, N+1)	The matrix that the pivot operations are carried out on
AC(N)	Activity of standards from library in SEDIT
ARR(N,64)	Matrix containing 64 channels of N standard spectra for residual calculation
B(N)	$C_j = \sum_i w_i a_{ij} x_i$
CC(N+1, N+1)	Correlation matrix for standards and sample
EF(N)	Logical variable to keep track of standard status in subroutine PIVOT
FP(N)	Partial F-value for output after pivot
FPM(N)	Partial F-to-add or F-to-remove
HA(N)	Half-life of standards from library in SEDIT
HAT(N)	Half-life of standard; printout order
IS(N)	Printout order of standards; OR in UEDIT can change during execution
ISL(N)	Printout order of standard; never changes during execution
IT(N)	Serial order of standards to be used in least-squares fit

PREGA (Cont'd)

MY(N) Integer vector used to check bit pattern of current set of standards for a particular standard; NOTE - values must also be added to DATA statement for MY

SS(N) Sum of counts over channels of standard spectra

STD(N) Standard error of nuclide concentration

TISO(2\*N),TISOT(2\*N) Names of standard nuclides

TST(N) Counting time of standard in seconds, from SEDIT

Z(N) Standard nuclide concentration

NOTE: For neatness of output, if the number of standards is increased the I/O statements for the correlation matrix at PREGA lines 204-208 and 248-252 must also be modified.

PIVOT

A(N+1, N+1) Matrix to be pivoted

E(N) Logical variable to determine which standards are in the current subset

## 8. PROGRAM SEDIT

### Operation

The standards editor program, SEDIT, is used to prepare a file that contains control parameters for the standards and the standard library for use by PREGA. The library contains information about the name, disk location, half-life, etc., about each standard spectrum. SEDIT writes to a file assigned to logical unit 9. SEDIT allows the user to build, change or list the standard control parameters, and to also create a new library, insert or delete a standard, append new standards or list the present library. The structure of the output file on logical unit 9 is given in the section under PREGA software organization. A listing of SEDIT is given in Appendix B.

### LANGUAGE

The program is written in DEC RT-11 FORTRAN.

### INPUTS

Keyboard	Logical unit 5, all operator interaction and input is from keyboard
Logical Unit 11	Output file of UEDIT used for reading number of standards wanted for fit, for one standard library listing option
Logical Unit 9	For modifying an existing SEDIT output file

### OUTPUT

Logical Unit 6	Record of operator interaction with SEDIT. This is usually defined as the keyboard unit the operator is using for input
File.Element	Logical unit 9 output file for SEDIT saved on disk for use with PREGA

A sample copy of the output from SEDIT is given in Appendix A.

## VARIABLES (SEDI)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
A(32)	Isotope name or file.element disk location
ACT	Activity of standard
ANS	Alphanumeric answer to SEDI prompt (e.g. Y, N)
BA	Background spectrum location FILE.ELEMENT (,DEVICE)
BB	= B, for build new header containing standard control parameters
BS	Background subtract option
BT	Counting time for background spectrum in seconds
CC	= C, to change one of the header parameters
D	Days, half-life unit
EDT	Program pointer
FNUM	REAL*4 I/O variable
H	Hours, half-life unit
HL	Standard half-life
I	Index for program control
IE	Final channel for computation
INT(26)	Used to rewrite library when inserting or deleting a standard
IS	Initial channel for computation
IT	Number of iterations NOTE - no longer used, set = 1
IVAR	Record number for direct-access I/O
K	Check time units of half-life and program pointer
L	Defines logical unit for output
LA	Switch program to append library mode
LD	Switch program to delete standard mode

VARIABLES (SEDI), (cont'd)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
LENGTH	Check for answer being carriage return only (to switch from header to library section or exit program)
LI	Switch program to insert standard mode
LN	Switch program to create a new library mode
LP	Switch program to list mode
LUI	Logical unit to read UEDIT variables NR and OR
LU	Logical unit for output file of SEDI
M	Total number of standards in library
MLA	NS from UEDIT for list standard option
MLI	OR from UEDIT for list standard option
MM	Months, half-life unit
N	Counter for number of standards in library
NC	Number of channels per standard
NUM	I*2 I/O variable
RC	Rejection coefficient no longer used, set = 1
SEC	Counting time of standard in seconds
Y	YES, I/O answer to SEDI prompt

## 9. PROGRAM UEDIT

### Operation

The unknown sample editor program, UEDIT, is used to prepare a file that contains control parameters and information about the sample for use by PREGA. UEDIT writes to a file assigned to logical unit 11. The program SEDIT also reads the UEDIT output file to control an operator option for listing the standard library. UEDIT allows the user to Build, Change, or List the output file with prompting questions. The structure of the output file on logical unit 11 is given in the section under PREGA software organization.

### LANGUAGE

The program is written in DEC RT-11 FORTRAN

### INPUTS

Keyboard	Logical unit 5, all operator interaction and input is from keyboard
Logical Unit 11	For modifying an existing UEDIT output file

### OUTPUTS

Logical Unit 6	Record of operator interaction with UEDIT. This is usually defined as the keyboard unit the operator is using for input
FILE.ELEMENT	Logical unit 11 output file for UEDIT saved on disk for use with SEDIT and PREGA

A sample copy of the output from UEDIT is given in Appendix A.

## VARIABLES (UEDIT)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
A(32)	FILE.ELEMENT location on disk of the unknown sample spectrum, background spectrum or residual spectrum
ANS	Alpha-numeric I/O variable
BA	Background spectrum disk location (FILE.ELEMENT (DEVICE))
BG	Background supplied option
BP	Pivot on background allowed option
BR	Start analysis with background only option
BS	Subtract background from sample option
BT	Counting time for background in seconds
CC	Switch program to change parameter mode
CRT	In logical unit number = 5
CT	Counting time of sample in seconds
DT	Decay time of sample, set = 1
EDT	Program pointer
F $\phi$	Rejection coefficient for partial F test
FNUM	R*4 I/O variable
GN	Gain shift ratio no longer used, set = 1
I	Index for loop over location of spectra
II	Index for program control
ITT	Upper bound of loop for output
IVAR	Record number for direct-access I/O to logical unit 11 file
K	Program control variable
LENGTH	Used as check for carriage return to exit current mode of program or exit program
LL	Switch program to list mode

## VARIABLES (UEDIT)

<u>NAME (DIMENSIONS)</u>	<u>USAGE</u>
LUN	Logical unit 11 for output
M	First record of LU 11 file
MF	Result multiplication factor option (usually set = 1)
NN	Switch program to create a new file mode
NO	N, the answer no to UEDIT prompt question
NS	Number of standards from library to be used in least-squares fit by PREGA
NUM	I*2 I/O variable
NUM1	Control variable for record number in LU-11 file
OR	Number of library standard in order of desired printout
RC	Rejection coefficient for rejection of standards used. No longer used.
RO	Output residuals option
RS	Residual spectrum disk location (FILE.ELEMENT (,DEVICE))
SB	Subtract background from standards option
TH	Threshold shift, no longer used. Set = 1
UN	Unknown spectrum disk location (FILE.ELEMENT (,DEVICE))
VR	Volume reduction factor option, usually set = 1
WD	Weighting factor determination option
WF	Weighting factor calculation option
YES	Y, the answer to a UEDIT prompt question

## PREGA - GENERAL OUTLINE

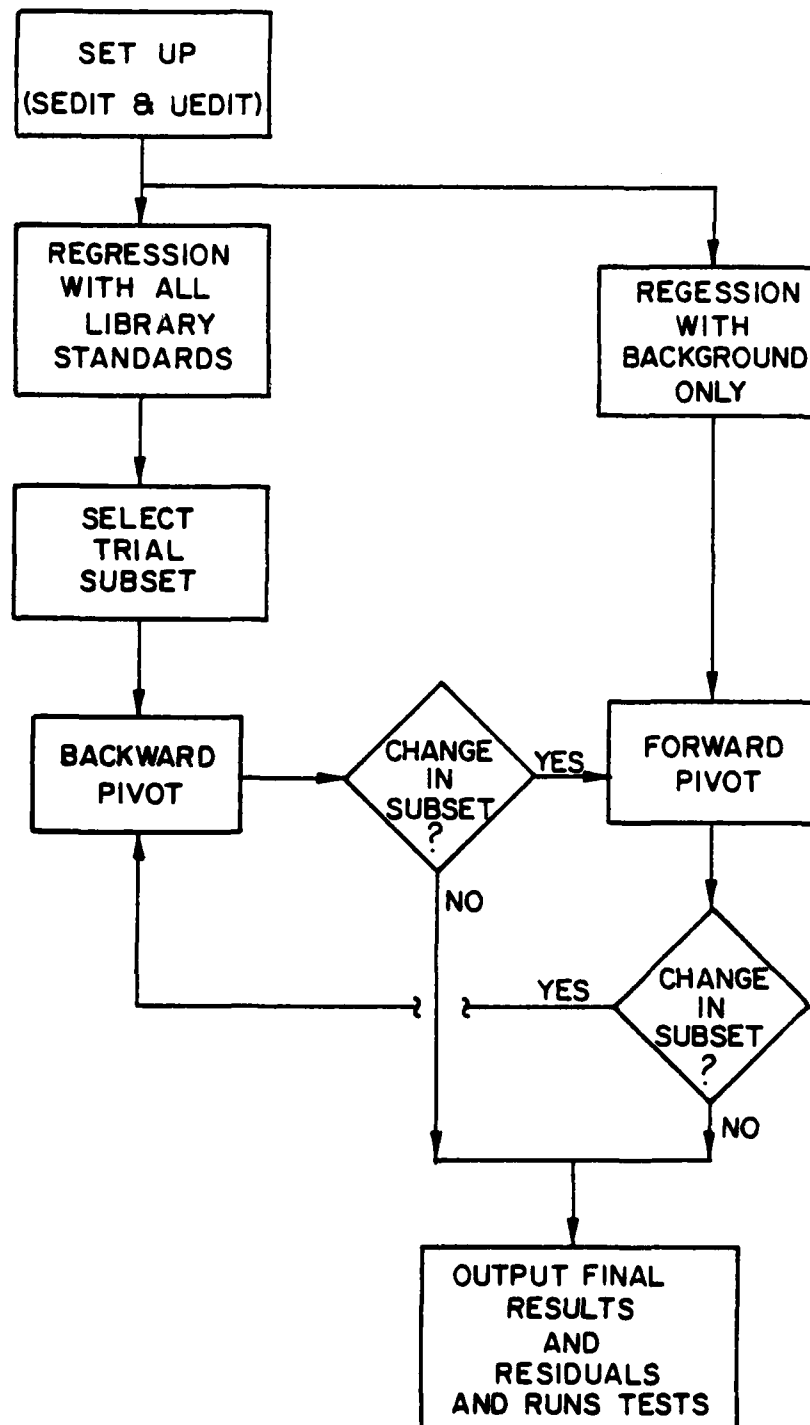


Figure 1. Summary flow chart of the program PREGA showing the major sections of the code.

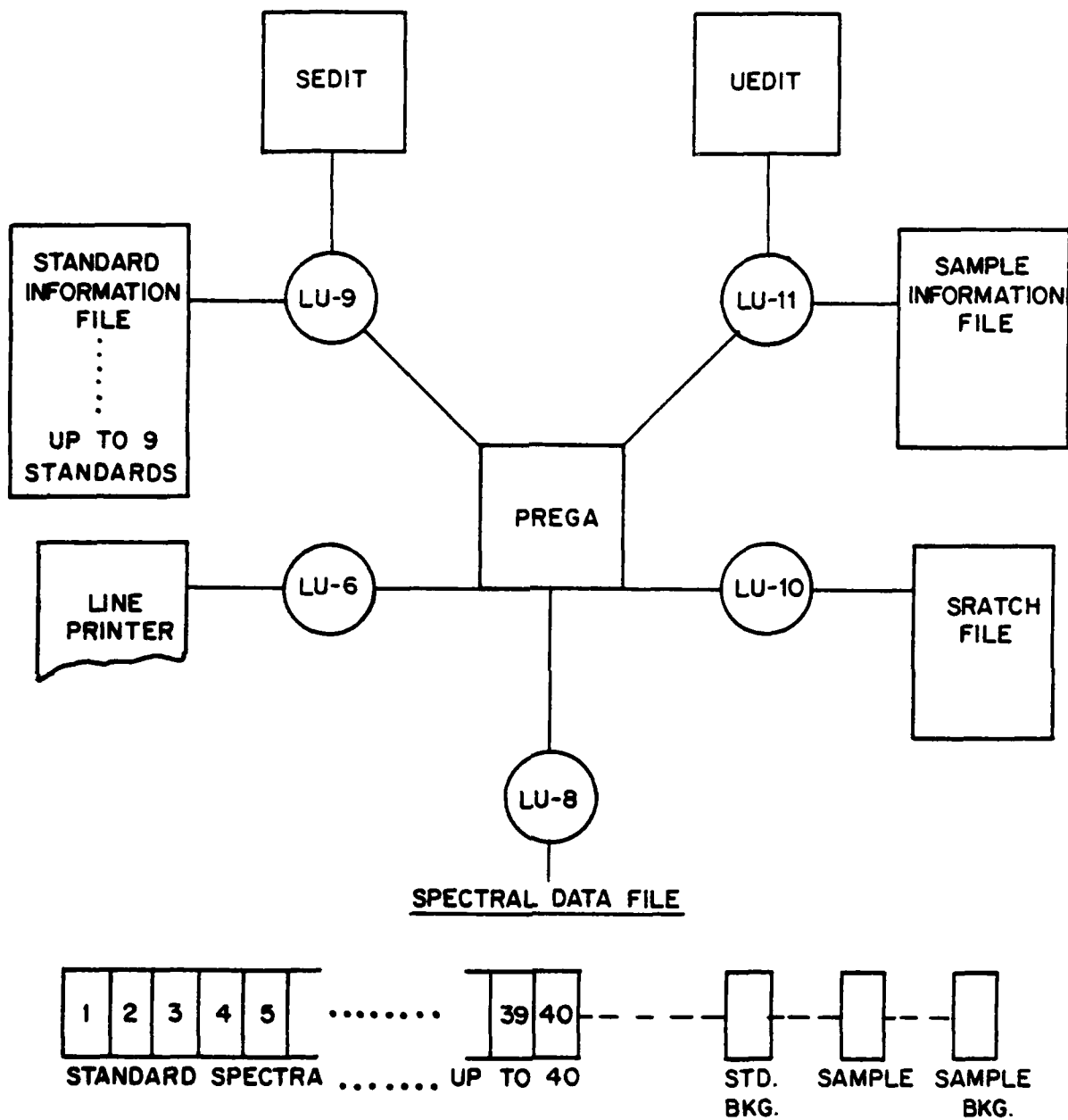


Figure 2. Logical unit and disk file structure for the program PREGA.

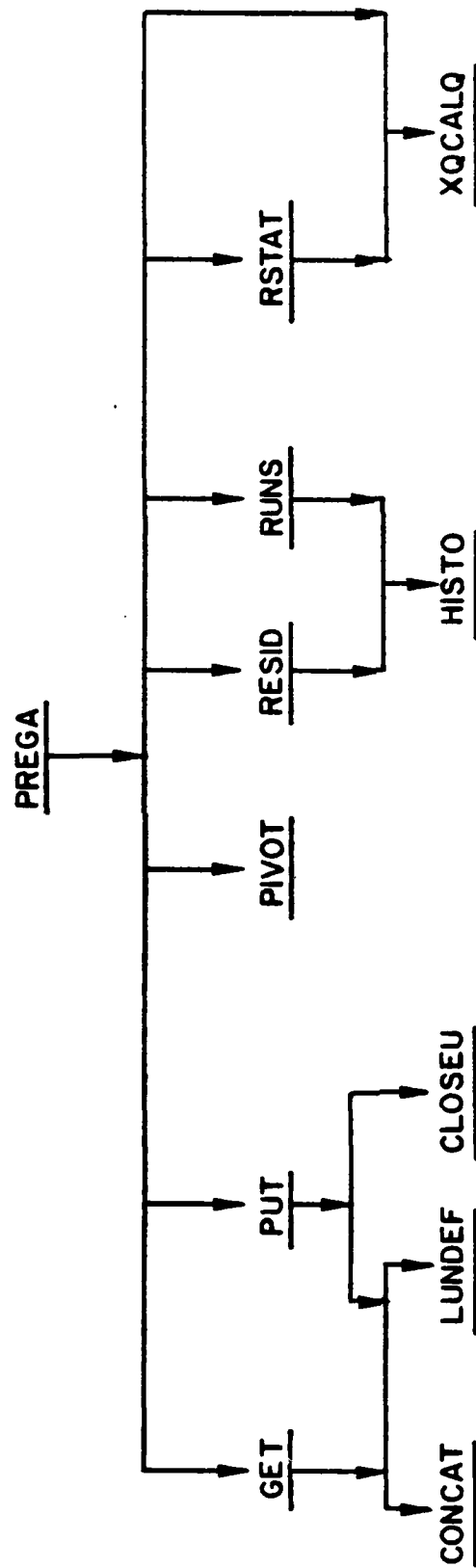


Figure 3. Hierarchy of subroutines called by the program PREGA.

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## APPENDIX A: Sample Output for PREGA

### Sample Output for Least Squares Analysis

The following pages contain sample outputs from the editor programs UEDIT and SEDIT, and from the program PREGA. The listing from UEDIT and SEDIT are provided to show the various options used in PREGA. The least squares analysis method used is the full PREGA mode. This mode uses a trial set of standards comprised of those standards which are most highly correlated with the unknown spectrum, as determined from a fit to the complete library.

PREGA UNKNOWN SAMPLE PARAMETERS

(UN) UNKNOWN SPECTRUM: FILE.ELEMENT(,DEVICE)  
: PREGA.G12161

(GN) GAIN SHIFT RATIO : 1.00000

(TH) THRESHOLD SHIFT : 1.00000

(BG) BACKGROUND SUPPLIED ? : Y

(BS) SUBTRACT BACKGROUND ? : Y

(BT) COUNTING TIME FOR BACKGROUND (SECS) : 390.000

(CT) COUNTING TIME FOR UNKNOWN SAMPLE : 430.000

(VR) VOLUME REDUCTION (OR INVERSE OF DILUTION)  
FACTOR : 1.00000

(DT) DECAY TIME : 0.000000

(MF) RESULT MULTIPLICATION FACTOR : 1.00000

(BA) BACKGROUND SPECTRUM: FILE.ELEMENT(,DEVICE)  
: PREGA.B12161

(WD) HOW ARE WEIGHTING FACTORS TO BE DETERMINED ?  
0: BASED ON ACTUAL COUNTS/CHANNEL.  
1: BASED ON CALCULATED COUNTS/CHN : 0

(NS) NUMBER OF ISOTOPES USED FROM THE STANDARD LIBRARY?: 6

(F0) F-TEST REJECTION COEFFICIENT.: 2.50000

(WF) WEIGHTING FACTOR CALCULATION.  
-1: (COUNTS)\*\*-1  
0: (SIGMA)\*\*-2  
1: 1 : 0

(RC) REJECTION COEFFICIENT APPLIED ? : Y

(BR) BACKGROUND REGRESSION ?  
0: TRIAL SET = CHOSEN STANDARDS  
1: TRIAL SET = BACKGROUND ONLY: 1

(BP) PIVOT ON BACKGROUND SPECTRUM ALLOWED?  
0: NO PIVOT ON BACKGROUND ALLOWED  
1: ALLOW PIVOT ON BACKGROUND SPECTRUM: 0

(RO) OUTPUT RESIDUALS ? : N

(RS) RESIDUAL SPECTRUM: FILE.ELEMENT(,DEVICE)  
: DDATB.R31020

(OR) NUMBER OF LIBRARY STANDARD IN ORDER OF DESIRED PRINTOUT  
: 1 2 3 4 5 7

PREGA LIBRARY HEADER

(NC) NUMBER OF CHANNELS PER STANDARD (MAX-512) : 255  
(IT) NUMBER OF ITERATIONS FOR THRESHOLD & GAIN CALC. : 1  
(BS) BACKGROUND SUBTRACT ? : N  
(IS) INITIAL CHANNEL FOR COMPUTATION : 19  
(IE) FINAL CHANNEL FOR COMPUTATION : 242  
(BT) COUNTING TIME OF BACKGROUND (SECS.) : 380.000  
(RC) REJECTION COEFFICIENT : 1.00000  
(BA) BACKGROUND SPECTRUM (FILE.ELEMENT(,DEVICE))  
: PREGA.812161

PREGA LIBRARY STANDARDS USED

STANDARD \* 1 : B12161  
FILE.ELEMENT(.DEVICE) : PREGA.B12161  
HALF-LIFE (SECS): 1.0000E 09  
COUNTING TIME OF STANDARD (SECS): 3.8000E 02  
ACTIVITY: 1.0000E 00

STANDARD \* 2 : 226RA  
FILE.ELEMENT(.DEVICE) : NAI.RA245  
HALF-LIFE (SECS): 1.0000E 09  
COUNTING TIME OF STANDARD (SECS): 1.4800E 03  
ACTIVITY: 1.0000E 00

STANDARD \* 3 : TH232  
FILE.ELEMENT(.DEVICE) : NAI.TH232  
HALF-LIFE (SECS): 1.0000E 09  
COUNTING TIME OF STANDARD (SECS): 1.0000E 03  
ACTIVITY: 1.0000E 00

STANDARD \* 4 : K40  
FILE.ELEMENT(.DEVICE) : NAI.K40  
HALF-LIFE (SECS): 1.0000E 09  
COUNTING TIME OF STANDARD (SECS): 1.0000E 03  
ACTIVITY: 1.0000E 00

STANDARD \* 5 : PC060  
FILE.ELEMENT(.DEVICE) : NAI.PC060  
HALF-LIFE (SECS): 1.0000E 09  
COUNTING TIME OF STANDARD (SECS): 3.8000E 02  
ACTIVITY: 1.0000E 00

STANDARD \* 7 : CS137  
FILE.ELEMENT(.DEVICE) : NAI.CS137  
HALF-LIFE (SECS): 1.0000E 09  
COUNTING TIME OF STANDARD (SECS): 1.0000E 03  
ACTIVITY: 1.0000E 00

# OUTPUT FOR PREGA ANALYSIS PROGRAM

SAMPLE SPECTRUM: PREGA.G12161

0.	0.	0.	0.	-1.	1.	153.
1620.	2227.	2427.	2644.	2579.	2669.	2451.
2238.	2447.	2079.	2254.	1918.	2065.	1680.
2007.	1396.	1423.	1278.	1179.	1397.	1145.
1062.	847.	970.	775.	959.	671.	547.
509.	667.	601.	660.	611.	517.	477.
472.	516.	311.	445.	520.	407.	344.
360.	335.	425.	388.	371.	277.	412.
313.	398.	339.	352.	404.	300.	356.
299.	260.	284.	336.	223.	292.	290.
337.	250.	265.	230.	276.	200.	252.
305.	213.	236.	166.	134.	269.	170.
126.	168.	249.	197.	203.	266.	123.
262.	216.	241.	210.	306.	358.	371.
376.	348.	280.	310.	233.	204.	168.
158.	170.	231.	242.	266.	232.	273.
243.	269.	139.	140.	159.	68.	76.
-26.	41.	44.	-14.	-36.	-15.	-43.
-48.	-64.	-23.	3.	-3.	-22.	2.
-15.	-28.	-9.	-17.	13.	-35.	-14.
-23.	-7.	9.	-7.	28.	9.	-27.
-16.	-10.	14.	-28.	9.	-16.	-22.
-21.	2.	24.	-9.	-16.	-4.	3.
-18.	4.	-14.	2.	-2.	15.	3.
-4.	14.	-0.	-17.	-16.	-4.	5.
10.	-10.	-13.	11.	21.	-30.	7.
-0.	-4.	-17.	-3.	4.	29.	-7.
-20.	-4.	16.	-0.	7.	-4.	22.
-13.	9.	2.	8.	3.	13.	-7.
7.	7.	2.	-3.	12.	4.	-7.
14.	-2.	17.	-17.	-13.	4.	4.
-10.	-24.	-23.	-24.	6.	-0.	-3.
-5.	1.	8.	1.	-4.	-18.	-3.
-15.	4.	2.	-0.	7.	-5.	-8.
0.	-8.	-2.	-9.	2.	-2.	2.
-6.	-3.	-5.	0.	-2.	-6.	-2.
-7.	-0.	-1.				

BACKGD SUM= 1.732E 05      SAMPLE SUM= 4.606E 04

\*\*\*\*\* CORRELATION MATRIX \*\*\*\*\*

	B12161	226RA	TH232	K40	PC060	CS137	G12161
B12161	1.0000	0.9533	0.8898	0.4003	0.8529	0.5202	0.8449
226RA		1.0000	0.7825	0.2955	0.8308	0.5252	0.8462
TH232			1.0000	0.3491	0.7614	0.4955	0.7405
K40				1.0000	0.3640	0.1447	0.3216
PC060					1.0000	0.4746	0.9555
CS137						1.0000	0.4954
G12161							1.0000

WEIGHTED SUMS OF STANDARDS AND UNKNOWN

8.7470E 01 9.4040E 01 7.0532E 02 4.3630E 01

9.4290E 01 1.0245E 02 0.0000E-01

# RESULTS OF FULL SET REGRESSION ON G12161

DEGREES OF FREEDOM= 218.  
 RSS= 4.513E 02  
 MSR= 2.070E 00

B12161	-4.3499E-02	+	2.85E-02	F=	2.3347E 00	Q=	9.3704E-01	X=	-1.5303E 00	RMSR=	2.0828E 00
226RA	1.6320E-01	+	4.56E-02	F=	1.2789E 01	Q=	1.4521E-04	X=	3.6256E 00	RMSR=	2.1816E 00
TH232	2.0187E-03	+	5.30E-03	F=	1.4523E-01	Q=	3.5171E-01	X=	3.8072E-01	RMSR=	2.0621E 00
K40	-8.9049E-03	+	1.64E-02	F=	2.9365E-01	Q=	7.0589E-01	X=	-5.4146E-01	RMSR=	2.0635E 00
PC060	1.2711E-01	+	5.47E-03	F=	5.3934E 02	Q=	0.0000E-01	X=	9.9999E 09	RMSR=	7.1591E 00
CS137	3.7913E-03	+	3.01E-03	F=	1.5861E 00	Q=	1.0378E-01	X=	1.2603E 00	RMSR=	2.0757E 00

# RESULTS OF TEST SET REGRESSION ON G12161

DEGREES OF FREEDOM= 220.  
 RSS= 4.524E 02  
 MSR= 2.057E 00

B12161	-3.9852E-02	+	1.77E-02	F=	5.0691E 00	Q=	9.8814E-01	X=	-2.2620E 00	RMSR=	2.0944E 00
226RA	1.6175E-01	+	3.68E-02	F=	1.9334E 01	Q=	3.5809E-06	X=	4.4918E 00	RMSR=	2.2271E 00
PC060	1.2698E-01	+	5.41E-03	F=	5.5020E 02	Q=	0.0000E-01	X=	9.9999E 09	RMSR=	7.1671E 00
CS137	4.0606E-03	+	2.96E-03	F=	1.8771E 00	Q=	8.5109E-02	X=	1.3714E 00	RMSR=	2.0647E 00

# RESULTS OF BACKWARD REGRESSION ON G12161

DEGREES OF FREEDOM= 221.  
 RSS= 4.563E 02  
 MSR= 2.065E 00

B12161	-3.8629E-02	+	1.77E-02	F=	4.7560E 00	Q=	9.8573E-01	X=	-2.1902E 00	RMSR=	2.0996E 00
226RA	1.6712E-01	+	3.66E-02	F=	2.0792E 01	Q=	1.5617E-06	X=	4.6658E 00	RMSR=	2.2487E 00
PC060	1.2740E-01	+	5.42E-03	F=	5.5352E 02	Q=	0.0000E-01	X=	9.9999E 09	RMSR=	7.2032E 00

## CALCULATED PARTIAL F-,Q- AND X-VALUES TO ADD:

TH232	F=	4.9604E-01	Q=	2.4075E-01	X=	7.0390E-01	RHO=	4.7431E-02	AMSR=	2.0694E 00
K40	F=	4.9536E-01	Q=	7.5909E-01	X=	-7.0342E-01	RHO=	-4.7398E-02	AMSR=	2.0694E 00

# RESULTS OF BACKWARD REGRESSION ON G12161

DEGREES OF FREEDOM= 221.  
 RSS= 4.563E 02  
 MSR= 2.065E 00

B12161	-3.8629E-02	+	1.77E-02	F=	4.7560E 00	Q=	9.8573E-01	X=	-2.1902E 00	RMSR=	2.0996E 00
226RA	1.6712E-01	+	3.66E-02	F=	2.0792E 01	Q=	1.5617E-06	X=	4.6658E 00	RMSR=	2.2487E 00
PC060	1.2740E-01	+	5.42E-03	F=	5.5352E 02	Q=	0.0000E-01	X=	9.9999E 09	RMSR=	7.2032E 00

## CALCULATED PARTIAL F-,Q- AND X-VALUES TO ADD:

TH232	F=	4.9604E-01	Q=	2.4075E-01	X=	7.0390E-01	RHO=	4.7431E-02	AMSR=	2.0694E 00
K40	F=	4.9536E-01	Q=	7.5909E-01	X=	-7.0342E-01	RHO=	-4.7398E-02	AMSR=	2.0694E 00
CS137	F=	1.8771E 00	Q=	8.5109E-02	X=	1.3714E 00	RHO=	9.1979E-02	AMSR=	2.0565E 00

\*\*\*\*\*  
 FINAL RESULT FOR G12161  
 \*\*\*\*\*

FIT= 2.073E 00

# RESULTS=CONCENTRATIONS AND EST STANDARD ERRORS

B12161	-3.0629E-02	+-	1.77E-02	F= 4.7560E 00	Q= 9.8573E-01	X= -2.1902E 00	RMSR= 2.0996E 00
226RA	1.6712E-01	+-	3.66E-02	F= 2.0792E 01	Q= 1.5617E-06	X= 4.6658E 00	RMSR= 2.2487E 00
PC060	1.2740E-01	+-	5.42E-03	F= 5.5352E 02	Q= 0.0000E-01	X= 9.9999E 09	RMSR= 7.2032E 00

## ANALYSIS OF VARIANCE

SOURCE	DF	SS	MS	F
REGRESN.	3.	5.510E 03	1.837E 03	8.096E 02
RESIDUAL	221.	4.563E 02	2.065E 00	
TOTAL	224.	5.966E 03		

\*\*\*\*\* LLNL R-STATISTIC \*\*\*\*\*

AUTO-CORRELATION COEFFICIENT.....	9.6947E-01
EXPECTATION VALUE.....	-1.3393E-02
STANDARD DEVIATION.....	6.7722E-02
EQUIVALENT NORMAL STANDARD DEVIATIONS.....	1.4513E 01
R-STAT FAP.....	0.0000E-01

## FINAL STATISTICS FOR ELIMINATED STANDARDS

TH232	F= 4.9604E-01	Q= 2.4075E-01	X= 7.0390E-01	RHO= 4.7431E-02	AMSR= 2.0694E 00
K40	F= 4.9536E-01	Q= 7.5910E-01	X= -7.0342E-01	RHO= -4.7398E-02	AMSR= 2.0694E 00
CS137	F= 1.0771E 00	Q= 8.5110E-02	X= 1.3714E 00	RHO= 9.1979E-02	AMSR= 2.0565E 00

# RATIO OF RESIDUALS OVER STD DEV PER CHANNEL FOR G12161

0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	-0.1	1.3	-0.4
2.5	-1.1	0.4	0.0	-0.2	2.2	0.3
0.1	-1.2	0.2	-1.9	0.8	-1.4	-2.4
-2.3	0.7	0.7	1.8	0.7	-0.2	-0.0
0.5	1.7	-1.2	1.1	2.1	1.0	-0.5
-0.1	-0.6	-0.0	-0.8	-1.1	-2.6	0.3
-0.8	1.9	0.7	1.3	2.2	0.5	1.7
0.6	-0.1	0.3	1.2	-1.2	0.4	0.7
1.9	0.2	0.5	-0.4	0.7	-1.1	0.4
1.6	-0.2	0.2	-1.2	-1.6	1.8	-0.4
-1.4	-0.0	2.1	0.7	1.2	2.8	-1.2
2.5	1.2	2.1	0.9	3.3	4.1	3.4
2.0	-0.6	-3.1	-1.7	-3.0	-2.0	-1.3
0.5	2.1	4.8	4.9	5.2	2.3	1.8
-0.8	-0.9	-5.2	-4.2	-2.0	-3.0	-1.1
-2.7	0.3	0.9	-0.6	-0.9	-0.3	-1.4
-1.4	-2.0	-0.7	0.4	0.2	-0.8	0.3
-0.7	-1.5	-0.5	-1.0	0.5	-2.1	-1.3
-1.5	-1.0	-0.4	-1.2	0.6	-0.3	-2.0
-1.4	-1.0	0.2	-1.9	0.1	-1.3	-1.4
-1.6	-0.1	1.8	-0.6	-1.2	-0.3	0.3
-1.1	0.5	-0.8	0.1	-0.2	1.2	0.3
-0.2	1.2	0.1	-0.9	-1.1	-0.3	0.3
0.7	-0.6	-0.8	0.7	1.5	-1.7	0.3
-0.1	-0.2	-1.1	-0.3	0.4	2.3	-0.4
-1.2	-0.4	1.4	0.1	0.7	-0.2	2.2
-1.1	0.7	0.2	0.8	0.3	1.2	-0.5
0.7	0.7	0.2	-0.2	1.0	0.4	-0.2
1.2	0.0	1.2	-0.8	-0.5	0.4	0.5
-0.3	-1.1	-1.3	-1.5	0.7	0.1	-0.1
-0.4	0.1	1.2	0.2	-0.4	-1.9	-0.3
-1.6	0.7	0.4	0.0	1.0	-0.7	-0.9
0.2	-1.0	-0.3	-1.1			

## SUSPICIOUS CHANNELS

97 4.10 108 4.79 109 4.91 110 5.24

MEAN RESIDUAL = -0.004, VARIANCE = 2.045, SKEWNESS = 0.376 , EXCESS = 1.87

# DISTRIBUTION OF RESIDUALS

SCALE FACTOR= 1

-5.00	1	*
-4.50	0	:
-4.00	1	*
-3.50	0	:
-3.00	3	***
-2.50	4	****
-2.00	8	*****
-1.50	18	*****
-1.00	33	*****
-0.500	28	*****
0.000	37	*****
0.500	42	*****
1.00	17	*****
1.50	7	****
2.00	14	*****
2.50	4	****
3.00	1	*
3.50	2	**
4.00	1	*
4.50	0	:
5.00	3	***

TOTAL = 224

# DISTRIBUTION OF RUNS

SCALE FACTOR= 1

-10.0	0	:
-9.00	0	:
-8.00	1	*
-7.00	2	**
-6.00	2	**
-5.00	0	:
-4.00	6	*****
-3.00	6	*****
-2.00	6	*****
-1.00	26	*****
0.000	0	:
1.00	20	*****
2.00	14	*****
3.00	6	*****
4.00	3	**
5.00	2	**
6.00	0	:
7.00	2	**
8.00	1	*
9.00	0	:
10.0	0	:

TOTAL = 97

# LOCATIONS AND SIZES OF LARGE RUNS

49	-7	58	7	69	5	92	8	100	-6
106	7	113	-8	123	-7	139	-6	198	5

Appendix B: FORTRAN Listings, DEC RT-11

1. PKANAL
2. PEAKNL
3. FREEFM
4. GSHIFT
5. REGAIN
6. RECHAN
7. SEDIT
8. UEDIT
9. PREGA
10. GET
11. HISTO
12. PIVOT
13. PUT
14. RESID
15. RSTAT
16. RUNS
17. XQCALC

```
C   PROGRAM PKANAL
C   WRITTEN BY G.W.PHILLIPS, JULY 1981
C
C   READS IN DATA FROM NUCLEAR DATA SPECTRAL FILES
C   AND CALCULATES PEAK POSITIONS, WIDTHS AND AREAS
C   FOR SELECTED REGIONS
C
C   INPUT: JL,JR - LOWER AND UPPER CHANNELS FOR PEAK REGIONS
C   ASC - FILENAME FOR SPECTRUM TO BE ANALYZED
C
C   OUTPUT: JL,JR - INPUT LIMITS FOR PEAK REGIONS
C   KL,KR - PEAK LIMITS (POSITIVE NET COUNT)
C   AMAX - PEAK MAXIMUM (NET COUNTS)
C   AREA - PEAK NET AREA
C   BKGD - BACKGROUND AREA BENEATH PEAK
C   CG - PEAK CENTROID
C   VAR - PEAK VARIANCE ABOUT CENTROID
C   FWHM - PEAK FULL WIDTH AT HALF MAXIMUM
C   ENERGY - CALIBRATED PEAK ENERGY
C
C   PROCEDURES CALLED:
C   PEAKNL - DOES PEAK ANALYSIS
C   GET - READS SPECTRUM AND ENERGY CALIBRATION FORD DISK
C
```

```
C
0001      COMMON/ARRAY/ARRAY(512)
0002      INTEGER CRT,DATA,PERIOD,BLANK,JL(20),JR(20)
0003      COMMON/DATA/DATA(80)/FREE/INTEG(16),REALX(16),ALPHA(16)
0004      REAL*8 ALPHA,ABLANK,AHEAD(11)
0005      LOGICAL*1 ASC(60)
0006      DATA ABLANK/8H
0007      DATA CRT/5/,LP/6/,IN/5/,IOUT/6/,PERIOD/1H./,BLANK/1H /,LUF/8/
0008      DATA AHEAD/8H REGION ,8H LIMITS ,8H PEAK ,8H LIMITS ,
1          8H HEIGHT ,8H AREA ,8H BKGD. ,
2          8H CENTROID,8H VARIANCE,8H FWHM ,
3          8H ENERGY /
C
0009 100   WRITE(CRT,110)
0010 110   FORMAT(1X,'ENTER REGIONS BY FIRST, LAST CHANNEL'/)
0011      DO 160 I=1,20
0012      READ(CRT,120)LEN,DATA
0013 120   FORMAT(Q,80A1)
0014      IF(LEN.LT.1) GOTO 180
0015      NX=2
0016      MX=1
0017      NA=1
0018      CALL FREEFM(NX,MX,NA,1)
0019      JL(I)=INTEG(1)
0020      JR(I)=INTEG(2)
0021      CONTINUE
0022 160   I=21
0023      N=I-1
0024 180   N=I-1
0025      IF(N.LT.1) GOTO 990
```

C

```
      C
      C
0027 200  IFORM=1
0028      WRITE(CRT,210)
0029 210  FORMAT(1H0,'FILENAME FOR SPECTRUM'/)
0030 220  READ(CRT,230)LEN,ASC
0031 230  FORMAT(Q,80A1)
0032      IF(LEN.LT.1) GOTO 990
0034      WRITE(IOUT,240) IFORM,(ASC(I),I=1,LEN)
0035 240  FORMAT(I1,80A1)
0036      IFORM=0
0037      WRITE(IOUT,250) AHEAD
0038 250  FORMAT(2X,4A0,1X,A0,6(4X,A0))
0039      MI=256
0040      CALL GET(ASC,ARRAY,IVAR,LUF,MI,A0,B0,C0)
0041      WRITE(CRT,260) MI
0042 260  FORMAT(1X,I5,' CHANNELS READ IN'/)
      C
      C
0043 300  DO 360 I=1,N
0044      KL=JL(I)
0045      KR=JR(I)
0046      CALL PEAKNL(KL,KR,ML,MR,MX,XL,XR,
1          AL,BL,AMAX,AREA,BKGD,CG,VAR,FWHM)
0047      ENERGY=A0+CG*(B0+CG*C0)
0048      WRITE(IOUT,320)JL(I),JR(I),KL,KR,AMAX,AREA,BKGD,
1          CG,VAR,FWHM,ENERGY
0049 320  FORMAT(2(I8,I6,2X),1X,7G12.4)
0050 360  CONTINUE
0051      GOTO 220
      C
0052 990  WRITE(IOUT,991)
0053 991  FORMAT(1H1)
0054      STOP
0055      END
```

# MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
JL	000006	INTEGER*2 ARRAY (20)
JR	000056	INTEGER*2 ARRAY (20)
AHEAD	000126	REAL*8 ARRAY (11)
ASC	000256	LOGICAL*1 ARRAY (60)
CRT	000362	INTEGER*2 VARIABLE
PERIOD	000372	INTEGER*2 VARIABLE
BLANK	000374	INTEGER*2 VARIABLE
ABLANK	000352	REAL*8 VARIABLE
LP	000364	INTEGER*2 VARIABLE
IN	000366	INTEGER*2 VARIABLE
IOUT	000370	INTEGER*2 VARIABLE
LUF	000376	INTEGER*2 VARIABLE
I	000630	INTEGER*2 VARIABLE
LEN	000632	INTEGER*2 VARIABLE
NX	000634	INTEGER*2 VARIABLE
MX	000636	INTEGER*2 VARIABLE
NA	000640	INTEGER*2 VARIABLE
FREEFM	000000	REAL*4 PROCEDURE
N	000642	INTEGER*2 VARIABLE
IFORM	000644	INTEGER*2 VARIABLE
MI	000646	INTEGER*2 VARIABLE
GET	000000	REAL*4 PROCEDURE
IVAR	000650	INTEGER*2 VARIABLE
A0	000652	REAL*4 VARIABLE
B0	000656	REAL*4 VARIABLE
C0	000662	REAL*4 VARIABLE
KL	000666	INTEGER*2 VARIABLE
KR	000670	INTEGER*2 VARIABLE
PEAKNL	000000	REAL*4 PROCEDURE
ML	000672	INTEGER*2 VARIABLE
MR	000674	INTEGER*2 VARIABLE
XL	000676	REAL*4 VARIABLE
XR	000702	REAL*4 VARIABLE
AL	000706	REAL*4 VARIABLE
BL	000712	REAL*4 VARIABLE
AMAX	000716	REAL*4 VARIABLE
AREA	000722	REAL*4 VARIABLE
BKGD	000726	REAL*4 VARIABLE
CG	000732	REAL*4 VARIABLE
VAR	000736	REAL*4 VARIABLE
FWHM	000742	REAL*4 VARIABLE
ENERGY	000746	REAL*4 VARIABLE
COMMON BLOCK /ARRAY/ LENGTH 004000		
ARRAY	000000	REAL*4 ARRAY (512)
COMMON BLOCK /DATA/ LENGTH 000240		
DATA	000000	INTEGER*2 ARRAY (80)
COMMON BLOCK /FREE/ LENGTH 000340		
INTEG	000000	INTEGER*2 ARRAY (16)
REALX	000040	REAL*4 ARRAY (16)
ALPHA	000140	REAL*8 ARRAY (16)

```
0001      SUBROUTINE PEAKNL(KL,KR,ML,MR,MX,XL,XR,  
1          AL,BL,AMAX,AREA,BKGD,CG,VAR,FWHM)  
C          WRITTEN BY G.W. PHILLIPS, JULY 1981  
C  
C          FINDS THE AREA, CENTER OF GRAVITY, VARIANCE AND FWHM  
C          FOR A PEAK IN A REGION BETWEEN KL AND KR  
C          AFTER SUBTRACTING A BACKGROUND CALCULATED  
C          AS A STRAIGHT LINE DRAWN BETWEEN  
C          THE MINIMUM BELOW THE PEAK AND THE MINIMUM  
C          ABOVE THE PEAK.  
C          IF THE DATA IS FLAT WITHIN STATISTICS AT THE MINIMUM  
C          THE AVERAGE OF THE THREE CHANNELS  
C          INCLUDING THE MINIMUM IS USED.  
C  
C          INPUT: KL,KR - INITIAL LIMITS FOR PEAK REGION  
C  
C          OUTPUT: KL,KR - FINAL LIMITS FOR PEAK (POSITIVE NET COUNT)  
C          ML,MR - MINIMUM CHANNELS BELOW AND ABOVE PEAK  
C          MX - PEAK MAXIMUM CHANNEL  
C          XL,XR - HALF MAXIMUM POINTS BELOW AND ABOVE PEAK  
C          AL,BL - SLOPE AND OFFSET (FROM ML)  
C                   FOR BACKGROUND  
C          AMAX - PEAK MAXIMUM (NET COUNTS)  
C          AREA - PEAK NET AREA  
C          BKGD - BACKGROUND AREA BENEATH PEAK  
C          CG - PEAK CENTROID  
C          VAR - PEAK VARIANCE ABOUT CENTROID  
C          FWHM - PEAK FULL WIDTH AT HALF MAXIMUM
```

```
      C
0002      COMMON/ARRAY/AX(512)
      D      DATA ICRT/5/
      C
      C      LOOK FOR MAXIMUM IN THE REGION
      C
0003 100      AMAX=0.
0004          MX=0
0005          DO 110 I=KL,KR
0006              IF(AMAX.GT.AX(I)) GOTO 110
0008              AMAX=AX(I)
0009              MX=I
0010 110      CONTINUE
      C
      C      LOOK FOR LOWER AND UPPER MINIMA
      C
0011          AMINL=AX(KL)
0012          ML=KL
0013          DO 130 I=KL,MX
0014              IF(AX(I).GT.AMINL) GOTO 130
0016              AMINL=AX(I)
0017              ML=I
0018 130      CONTINUE
0019          AMINR=AX(MX)
0020          MR=MX
0021          DO 140 I=MX,KR
0022              IF(AX(I).GE.AMINR) GOTO 140
0024              AMINR=AX(I)
0025              MR=I
0026 140      CONTINUE
```

```
C
C      DETERMINE BACKGROUND PARAMETERS
C
0027 200  IF(ML.EQ.KL) ML=ML+1
0029      J=ML-1
0030      K=ML+1
0031      SUML=0.
0032      SQL=0.
0033      DO 210 I=J,K
0034      FL=AX(I)
0035      SUML=SUML+FL
0036      SQL=SQL+FL**2
0037 210  CONTINUE
0038      IF(MR.EQ.KR) MR=MR-1
0040      J=MR-1
0041      K=MR+1
0042      SUMR=0.
0043      SQR=0.
0044      DO 220 I=J,K
0045      FR=AX(I)
0046      SUMR=SUMR+FR
0047      SQR=SQR+FR**2
0048 220  CONTINUE
0049      DL=AMAX1(ABS(AX(ML-1)-AX(ML)),ABS(AX(ML+1)-AX(ML)))
0050      DR=AMAX1(ABS(AX(MR-1)-AX(MR)),ABS(AX(MR+1)-AX(MR)))
0051      AL=SUML/3.
0052      IF(DL.LT.2.*SQL) GOTO 240
0054      IF(AX(ML).GT.AX(ML-1)) ML=ML-1
0056      AL=AX(ML)
0057 240  AR=SUMR/3.
0058      IF(DR.LT.2.*SQR) GOTO 250
0060      IF(AX(MR).GT.AX(MR+1)) MR=MR+1
0062      AR=AX(MR)
0063 250  BL=(AR-AL)/FLOAT(MR-ML)
D      WRITE(ICRT,260)ML,MR,AL,BL
D260  FORMAT(1X,'BACKGROUND PARAMETERS: ML MR AL BL'/
D      1      1X,2I5,2G12.4)
C
C      LOOK FOR MAXIMUM IN NET COUNTS
C
0064      MX=ML
0065      AMAX=AX(ML)-AL
0066      DO 270 I=ML,MR
0067      A=AX(I)-AL-BL*FLOAT(I-ML)
0068      IF(A.LT.AMAX) GOTO 270
0070      AMAX=A
0071      MX=I
0072 270  CONTINUE
C
```

```
C
C   DEFINE PEAK LIMITS
C
0073 300 KL=ML-1
0074      DO 310 I=ML,MX
0075      IF(AX(I).LT.AL+BL*FLOAT(I-ML)) KL=I
0077 310 CONTINUE
0078      KL=MIN0(KL+1,MX)
0079      KR=MX
0080      DO 320 I=MX,MR
0081      IF(AX(I).LT.AL+BL*FLOAT(I-ML)) GOTO 330
0083      KR=I
0084 320 CONTINUE
C
C   CALCULATE PEAK PARAMETERS
C
0085 330 AI=0.
0086      AISQ=0.
0087      AREA=0.
0088      BKGD=0.
0089      CG=0.
0090      VAR=0.
0091      FWHM=0.
D      WRITE(ICRT,340)
D340  FORMAT(4X,'I',3X,' COUNTS ',3X,' BKGD. ',3X,' NET ',
D      1      3X,' AREA ',3X,' AI ',3X,' AISQ ')
0092      DO 360 I=KL,KR
0093      B=AL+BL*FLOAT(I-ML)
0094      BKGD=BKGD+B
0095      A=AX(I)-B
0096      AREA=AREA+A
0097      AI=AI+A*FLOAT(I)
0098      AISQ=AISQ+A*FLOAT(I)**2
D      WRITE(ICRT,350)I,AX(I),B,A,AREA,AI,AISQ
D350  FORMAT(1X,I4,6G11.3)
0099 360 CONTINUE
0100      IF(AREA.EQ.0.) RETURN
0102      CG=AI/AREA
0103      VAR=(AISQ+AREA*CG**2-2.*AI*CG)/AREA
```

```
C
C      FIND FWHM
C
0104 400  AHALF=AMAX/2.
0105      B=AL+BL*FLOAT(KL-ML-1)
0106      AO=AX(KL-1)-B
0107      DO 410 I=KL,MX
0108      IL=I
0109      B=B+BL
0110      A=AX(I)-B
0111      IF(A.GT.AHALF) GOTO 420
0113      AO=A
0114 410  CONTINUE
0115 420  DA=A-AO
0116      IF(DA.EQ.0.) DA=2.*(A-AHALF)
0118      X=(A-AHALF)/DA
0119      XL=FLOAT(IL)-X
C
0120      B=AL+BL*FLOAT(MX-ML-1)
0121      AO=AX(MX-1)-B
0122      DO 430 I=MX,KR
0123      IR=I
0124      B=B+BL
0125      A=AX(I)-B
0126      IF(A.LT.AHALF) GOTO 440
0128      AO=A
0129 430  CONTINUE
0130      IR=IR+1
0131 440  DA=AO-A
0132      IF(DA.EQ.0.) DA=2.*(AHALF-A)
0134      X=(AHALF-A)/DA
0135      XR=FLOAT(IR)-X
0136      FWHM=XR-XL
D      WRITE(ICRT,450) MX,IL,IR,XL,XR,FWHM
D450  FORMAT(1X,'WIDTH PARAMETERS: MX IL IR XL XR FWHM' /
D      1      1X,3I8,3G12.4/)
C
0137      RETURN
0138      END
```

# MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
KL	000014	INTEGER*2 PARAMETER VARIABLE
KR	000016	INTEGER*2 PARAMETER VARIABLE
ML	000020	INTEGER*2 PARAMETER VARIABLE
MR	000022	INTEGER*2 PARAMETER VARIABLE
MX	000024	INTEGER*2 PARAMETER VARIABLE
XL	000026	REAL*4 PARAMETER VARIABLE
XR	000030	REAL*4 PARAMETER VARIABLE
AL	000032	REAL*4 PARAMETER VARIABLE
BL	000034	REAL*4 PARAMETER VARIABLE
AMAX	000036	REAL*4 PARAMETER VARIABLE
AREA	000040	REAL*4 PARAMETER VARIABLE
BKGD	000042	REAL*4 PARAMETER VARIABLE
CG	000044	REAL*4 PARAMETER VARIABLE
VAR	000046	REAL*4 PARAMETER VARIABLE
FUHM	000050	REAL*4 PARAMETER VARIABLE
I	000052	INTEGER*2 VARIABLE
AMINL	000054	REAL*4 VARIABLE
AMINR	000060	REAL*4 VARIABLE
J	000064	INTEGER*2 VARIABLE
K	000066	INTEGER*2 VARIABLE
SUML	000070	REAL*4 VARIABLE
SQL	000074	REAL*4 VARIABLE
FL	000100	REAL*4 VARIABLE
SUMR	000104	REAL*4 VARIABLE
SQR	000110	REAL*4 VARIABLE
FR	000114	REAL*4 VARIABLE
DL	000120	REAL*4 VARIABLE
AMAX1	000000	REAL*4 PROCEDURE
ABS	000000	REAL*4 PROCEDURE
DR	000124	REAL*4 VARIABLE
AR	000130	REAL*4 VARIABLE
FLOAT	000000	REAL*4 PROCEDURE
A	000134	REAL*4 VARIABLE
MIN0	000000	INTEGER*2 PROCEDURE
AI	000140	REAL*4 VARIABLE
AIQ	000144	REAL*4 VARIABLE
B	000150	REAL*4 VARIABLE
AHALF	000154	REAL*4 VARIABLE
AO	000160	REAL*4 VARIABLE
IL	000164	INTEGER*2 VARIABLE
DA	000166	REAL*4 VARIABLE
X	000172	REAL*4 VARIABLE
IR	000176	INTEGER*2 VARIABLE

COMMON BLOCK /ARRAY/      LENGTH 004000

```

0001 SUBROUTINE FREEFM(N,M,NA,ITYPE)
      LAST REVISED AUGUST 1981 BY G.W.P.
      C
      C
      C GENERAL SUBROUTINE TO DECODE DATA READ IN FREE FIELD FORMAT
      C DELIMITERS ARE EITHER A BLANK OR A COMMA
      C THE ROUTINE ASSUMES THE DATA HAS BEEN READ INTO ARRAY IDATA WITH
      C THE FORMAT (80A1)
      C N IS THE NUMBER OF DATA ELEMENTS. MAXIMUM=16
      C N IS RETURNED AS THE NUMBER OF DATA ELEMENTS FOUND
      C M IS THE LOCATION IN THE ARRAY FOR STORING THE FIRST DATA ELEMENT
      C M IS RETURNED AS THE LOCATION FOLLOWING THE NTH DATA ELEMENT
      C NA IS THE BEGINNING COLUMN OF THE DATA
      C NA IS RETURNED AS THE COLUMN FOLLOWING THE NTH DATA ELEMENT
      C ITYPE IS THE TYPE OF DATA,
      C 1=INTEGER
      C 2=REAL
      C 3=ALPHANUMERIC
      C
0002 COMMON/DATA/IDATA(80)
0003 COMMON/FREE/INTEG(16),REALX(16),ALPHA(16)
0004 INTEGER SEMI,E,COMMA
0005 REAL*8 ALPHA,BLANK
0006 DIMENSION ITEMP(20),AFORM(2)
0007 DATA SEMI,E,IBLK1,COMMA,IBLK2,BLNK4,BLANK
      * /','E',' ',' ',' ',' ',' ',' ',' ',' ',' ',' ',' ',' ',' /
      C
0008 L=M
0009 M=M+N-1
0010 DO 300 I=L,M
0011 IF(NA.GT.80) GO TO 400
      C
      C LOOK FOR START OF CURRENT FIELD
      C
0013 DO 210 J=NA,80
0014 JQQ=J
0015 IF(IDATA(J).NE.IBLK1) GO TO 215
0017 210 CONTINUE
0018 NA=81
0019 GO TO 400
0020 215 IF(IDATA(JQQ).NE.COMMA) GO TO 220
0022 NA=JQQ+1
0023 GO TO 290

```

```
C
C   LOOK FOR END OF CURRENT FIELD
C
0024 220 IL=JQQ
0025      ILQ = IL
0026 221 DO 230 J=ILQ,80
0027      JQQ=J
0028      IF(IDATA(J).EQ.IBLK1) GO TO 235
0030      IF(IDATA(J).NE.COMMA) GO TO 230
0032      IR=J-1
0033      NA=J+1
0034      GO TO 250
0035 230 CONTINUE
0036      IR=80
0037      NA=81
0038      GO TO 250

C
C   CHECK FOR EXPONENT
C
0039 235 IF((ITYPE.NE.2).OR.(IDATA(JQQ-1).NE.E)) GO TO 236
0041      ILQ = JQQ + 1
0042      GO TO 221
0043 236 IR=JQQ - 1
0044      IJ=JQQ+1

C
C   SET NA TO START OF NEXT FIELD
C
0045      DO 240 J=IJ,80
0046      IF(IDATA(J).EQ.IBLK1) GO TO 240
0048      NA=J
0049      IF(IDATA(J).EQ.COMMA) NA=NA+1
0051      GO TO 250
0052 240 CONTINUE
0053      NA=81

C
C   ENCODE DATA IN CURRENT FIELD
C
0054 250 NI=IR-IL+1
0055      IF(NI.LT.1) GO TO 290
0057      ENCODE(NI,255,ITEMP) (IDATA(J),J=IL,IR)
0058 255 FORMAT(83A1)
```

```
C
C
0059      GO TO (260,270,280), ITYPE
C
C      DECODE INTEGER DATA
C
0060      260 ENCODE(8,265,AFORM) NI
0061      265 FORMAT('I12,')
0062      DECODE(NI,AFORM,ITEMP) INTEG(I)
0063      GO TO 300
C
C      DECODE REAL DATA
C
0064      270 ENCODE(8,275,AFORM) NI
0065      275 FORMAT('E12,.0')
0066      DECODE(NI,AFORM,ITEMP) REALX(I)
0067      GO TO 300
C
C      DECODE ALPHANUMERIC DATA
C
0068      280 IF(NI.GT.8) NI=8
0070      DO 287 J=1,NI
0071      IF(ITEMP(J).EQ.SEMI) ITEMP(J)=COMMA
0073      287 CONTINUE
0074      ENCODE(8,288,AFORM) NI
0075      288 FORMAT('A11,')
0076      DECODE(8,AFORM,ITEMP) ALPHA(I)
0077      GO TO 300
C
C      BLANK OUT REMAINING DATA
C
0078      290 INTEG(I)=IBLK2
0079      REALX(I)=BLNK4
0080      ALPHA(I)=BLANK
0081      300 CONTINUE
0082      M=M+1
0083      RETURN
C
C      BLANK INPUT, BLANK OUT ALL DATA
C
0084      400 DO 410 J=1,M
0085      INTEG(J)=IBLK2
0086      REALX(J)=BLNK4
0087      ALPHA(J)=BLANK
0088      410 CONTINUE
0089      M=1
0090      N=M-L
0091      RETURN
0092      END
```

# MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
ITEMP	000024	INTEGER*2 ARRAY (20)
AFORM	000074	REAL*4 ARRAY (2)
N	000014	INTEGER*2 PARAMETER VARIABLE
M	000016	INTEGER*2 PARAMETER VARIABLE
NA	000020	INTEGER*2 PARAMETER VARIABLE
ITYPE	000022	INTEGER*2 PARAMETER VARIABLE
SEMI	000104	INTEGER*2 VARIABLE
E	000106	INTEGER*2 VARIABLE
COMMA	000112	INTEGER*2 VARIABLE
BLANK	000122	REAL*8 VARIABLE
IBLK1	000110	INTEGER*2 VARIABLE
IBLK2	000114	INTEGER*2 VARIABLE
BLNK4	000116	REAL*4 VARIABLE
L	000210	INTEGER*2 VARIABLE
I	000212	INTEGER*2 VARIABLE
J	000214	INTEGER*2 VARIABLE
JQQ	000216	INTEGER*2 VARIABLE
IL	000220	INTEGER*2 VARIABLE
ILQ	000222	INTEGER*2 VARIABLE
IR	000224	INTEGER*2 VARIABLE
IJ	000226	INTEGER*2 VARIABLE
NI	000230	INTEGER*2 VARIABLE

COMMON BLOCK /DATA/      LENGTH 000240

IDATA    000000    INTEGER\*2 ARRAY (80)

COMMON BLOCK /FREE/      LENGTH 000340

INTEG	000000	INTEGER*2 ARRAY (16)
REALX	000040	REAL*4 ARRAY (16)
ALPHA	000140	REAL*8 ARRAY (16)

```
C      PROGRAM GSHIFT
C      WRITTEN BY G.W.PHILLIPS, AUGUST 1981
C
C      READS IN DATA FROM NUCLEAR DATA SPECTRAL FILES
C      AND PERFORMS A GAIN AND ZERO OFFSET ADJUSTMENT
C
0001      DIMENSION S(256),R(256)
0002      INTEGER CRT,DATA,PERIOD,BLANK
0003      COMMON/DATA/ DATA(80)/FREE/INTEG(16),REALX(16),ALPHA(16)
0004      COMMON/HEAD/ IHDR,TITLE(32),ID(8),ELTIME,PLTIME,ERTIME,PRTIME
0005      INTEGER*2 TITLE,ID,DUMT(32),DUMID(8)
0006      REAL*8 ALPHA,ABLANK,AHEAD(10)
0007      LOGICAL*1 ASC(60),YES
0008      DATA CRT/5/,LP/6/,IN/5/,IOUT/6/,PERIOD/1H./,BLANK/1H /,LUF/8/
0009      DATA AHEAD/8H REGION ,8H LIMITS ,8H  PEAK ,8H LIMITS ,
1          8H HEIGHT ,8H AREA ,8H  BKGD. ,
2          8H CENTROID,8H VARIANCE,8H  FWHM /
0010      DATA BLNK4/4H      /,ABLANK/8H      /,YES/1HY/
```

```
      C
      C
0011 100 WRITE(CRT,110)
0012 110 FORMAT(1H0,'FILENAME FOR SPECTRUM'//)
0013      READ(CRT,120)LEN,ASC
0014 120 FORMAT(Q,80A1)
0015      IF(LEN.LT.1) GOTO 990
0017      LUF=8
0018      NCH=256
0019      CALL GET(ASC,R,IVAR,LUF,NCH,A0,B0,C0)
0020      WRITE(CRT,130) NCH
0021 130 FORMAT(1X,15,' CHANNELS READ IN'//)
      D
      D140 WRITE(IOUT,140)(R(I),I=1,NCH)
      D140 FORMAT(1H1,10G12.3/(1X,10G12.3))
      D
      D150 WRITE(IOUT,150)
      D150 FORMAT(1H1)
0022      WRITE(CRT,160)B0,A0,C0
0023 160 FORMAT(1X,'ENERGY CALIBRATION FROM HEADER GIVES SLOPE,OFFSET,'
      1      'CURVATURE:'/3G12.4/
      2      1X,'USE THIS FOR OLD SLOPE AND OFFSET, YES OR NO?'//)
0024      READ(CRT,170)LEN,ASC
0025 170 FORMAT(Q,80A1)
0026      IF(LEN.LT.1) GOTO 200
0028      IF(ASC(1).EQ.YES) GOTO 300
      C
      C
0030 200 A0=0.
0031      B0=1.
0032      C0=0.
0033      WRITE(CRT,210)
0034 210 FORMAT(1X,'ENTER OLD SLOPE,OFFSET'//)
0035      READ(CRT,220)LEN,DATA
0036 220 FORMAT(Q,80A1)
0037      IF(LEN.LT.1) GOTO 300
0039      NX=2
0040      MX=1
0041      NA=1
0042      CALL FREEFM(NX,MX,NA,2)
0043      IF(REALX(1).NE.BLNK4) B0=REALX(1)
0045      IF(REALX(2).NE.BLNK4) A0=REALX(2)
0047 300 DO 230 I=1,32
0048      DUMT(I)=TITLE(I)
0049 230 CONTINUE
0050      DO 235 I=1,8
0051      DUMID(I)=ID(I)
0052 235 CONTINUE
0053      IDELT=ELTIME
0054      IDPLT=PLTIME
0055      IDERT=ERTIME
0056      IDPRT=PRTIME
```

```
      C
      C
0057      WRITE(CRT,310)
0058 310  FORMAT('0TO GET NEW SLOPE AND OFFSET FROM SPECTRAL FILE'//
      1      ' ENTER FILENAME'$)
0059      READ(CRT,320)LEN,ASC
0060 320  FORMAT(Q,80A1)
0061      IF(LEN.LT.1) GOTO 350
0063      KUF=8
0064      MCH=256
0065      CALL GET(ASC,S,JVAR,KUF,MCH,A1,B1,C1)
0066      WRITE(CRT,330)B1,A1,C1
0067 330  FORMAT(' HEADER GIVES SLOPE,OFFSET,CURVATURE:'//3F12.7//
      1      ' USE THIS FOR NEW AND OFFSET, YES OR NO?'//)
0068      READ(CRT,340) LEN,ASC
0069 340  FORMAT(Q,80A1)
0070      IF(LEN.LT.1) GOTO 350
0072      IF(ASC(1).EQ.YES) GOTO 400
      C
0074 350  A1=0.
0075      B1=1.
0076      C1=0.
0077      WRITE(CRT,355)
0078 355  FORMAT(1X,'ENTER NEW SLOPE,OFFSET'//)
0079      READ(CRT,360)LEN,DATA
0080 360  FORMAT(Q,80A1)
0081      IF(LEN.LT.1) GOTO 370
0083      NX=2
0084      MX=1
0085      NA=1
0086      CALL FREEFM(NX,MX,NA,2)
0087      IF(REALX(1).NE.BLNK4) B1=REALX(1)
0089      IF(REALX(2).NE.BLNK4) A1=REALX(2)
0091      GOTO 400
      C
0092 370  G=1.
0093      EPS=0.
0094      WRITE(CRT,380)
0095 380  FORMAT(1X,'ENTER GAIN,ZERO SHIFT'//)
0096      READ(CRT,390)LEN,DATA
0097 390  FORMAT(Q,80A1)
0098      IF(LEN.LT.1) GOTO 990
0100      NX=2
0101      MX=1
0102      NA=1
0103      CALL FREEFM(NX,MX,NA,2)
0104      IF(REALX(1).NE.BLNK4) G=REALX(1)
0106      IF(REALX(2).NE.BLNK4) EPS=REALX(2)
0108      GOTO 411
```

```
C
C
C      PERFORM GAIN SHIFT
C
0109 400  G=B0/B1
0110      EPS=(A0-A1)/B1
0111      WRITE(CRT,410) G, EPS
0112 410  FORMAT(1H0, 'RESULTING GAIN AND ZERO SHIFT ARE: '/2G12.4/)
0113 411  MF=1
0114      MR=NCH
0115      CALL REGAIN(R,S,G, EPS, MR, MF, NCH)
0116      CALL RECHAN(R,S, MR, MF, NCH)
D      WRITE(IOUT,412)(R(I), I=1, NCH)
D412  FORMAT(1X, 10G12.3)
D      WRITE(IOUT,414)
D414  FORMAT(1H1)
0117      WRITE(CRT,420)
0118 420  FORMAT(1X, 'FILENAME FOR OUTPUT SPECTRUM' /)
0119      READ(CRT,430) LEN, ASC
0120 430  FORMAT(Q, 80A1)
0121      IF(LEN.LT.1) GOTO 990
0123      DO 440 I=1, 32
0124      TITLE(I)=DUMT(I)
0125 440  CONTINUE
0126      DO 445 I=1, 8
0127      ID(I)=DUMID(I)
0128 445  CONTINUE
0129      ELTIME=IDELT
0130      PLTIME=IDPLT
0131      ERTIME=IDERT
0132      PRTIME=IDPRT
0133      CALL PUT(ASC, R, IVAR, LUF, NCH, A1, B1, C1)
C
0134 990  STOP
0135      END
```

## MIDAS FORTRAN IV STORAGE MAP

COMMON BLOCK /FREE/

LENGTH 000340

NAME	OFFSET	ATTRIBUTES
S	000006	REAL*4 ARRAY (256)
R	002006	REAL*4 ARRAY (256)
DUMT	004006	INTEGER*2 ARRAY (32)
DUMID	004106	INTEGER*2 ARRAY (8)
AHEAD	004126	REAL*8 ARRAY (10)
ASC	004246	LOGICAL*1 ARRAY (60)
CRT	004342	INTEGER*2 VARIABLE
PERIOD	004352	INTEGER*2 VARIABLE
BLANK	004354	INTEGER*2 VARIABLE
ABLANK	004364	REAL*8 VARIABLE
YES	004374	LOGICAL*1 VARIABLE
LP	004344	INTEGER*2 VARIABLE
IN	004346	INTEGER*2 VARIABLE
IOUT	004350	INTEGER*2 VARIABLE
LUF	004356	INTEGER*2 VARIABLE
BLNK4	004360	REAL*4 VARIABLE
LEN	005424	INTEGER*2 VARIABLE
NCH	005426	INTEGER*2 VARIABLE
GET	000000	REAL*4 PROCEDURE
IVAR	005430	INTEGER*2 VARIABLE
A0	005432	REAL*4 VARIABLE
B0	005436	REAL*4 VARIABLE
C0	005442	REAL*4 VARIABLE
NX	005446	INTEGER*2 VARIABLE
MX	005450	INTEGER*2 VARIABLE
NA	005452	INTEGER*2 VARIABLE
FREEFM	000000	REAL*4 PROCEDURE
I	005454	INTEGER*2 VARIABLE
IDELT	005456	INTEGER*2 VARIABLE
IDPLT	005460	INTEGER*2 VARIABLE
IDERT	005462	INTEGER*2 VARIABLE
IDPRT	005464	INTEGER*2 VARIABLE
KUF	005466	INTEGER*2 VARIABLE
MCH	005470	INTEGER*2 VARIABLE
JVAR	005472	INTEGER*2 VARIABLE
A1	005474	REAL*4 VARIABLE
B1	005500	REAL*4 VARIABLE
C1	005504	REAL*4 VARIABLE
G	005510	REAL*4 VARIABLE
EPS	005514	REAL*4 VARIABLE
MF	005520	INTEGER*2 VARIABLE
MR	005522	INTEGER*2 VARIABLE
REGAIN	000000	REAL*4 PROCEDURE
RECHAN	000000	REAL*4 PROCEDURE
PUT	000000	REAL*4 PROCEDURE

COMMON BLOCK /DATA/ LENGTH 000240

DATA 000000 INTEGER\*2 ARRAY (80)

# MIDAS FORTRAN IV STORAGE MAP

NAME      OFFSET    ATTRIBUTES

COMMON BLOCK /HEAD/      LENGTH 000142

IHDR	000000	INTEGER*2	VARIABLE
TITLE	000002	INTEGER*2	ARRAY (32)
ID	000102	INTEGER*2	ARRAY (8)
ELTIME	000122	REAL*4	VARIABLE
PLTIME	000126	REAL*4	VARIABLE
ERTIME	000132	REAL*4	VARIABLE
PRTIME	000136	REAL*4	VARIABLE
AL*4		PROCEDURE	
A	000134	REAL*4	VARIABLE
MIN0	000000	INTEGER*2	PROCEDURE
AI	000140	REAL*4	VARIABLE
AISO	000144	REAL*4	VARIABLE
B	000150	REAL*4	VARIABLE
AHALF	000154	REAL*4	VARIABLE
AO	000160	REAL*4	VARIABLE

AD-A141 539

PROGRAM PREGA PIVOTAL REGRESSION ANALYSIS OF GAMMA-RAY  
SPECTRA FROM NAI(T. (U) NAVAL RESEARCH LAB WASHINGTON  
DC G W PHILLIPS ET AL. 06 APR 84 NRL-MR-5275

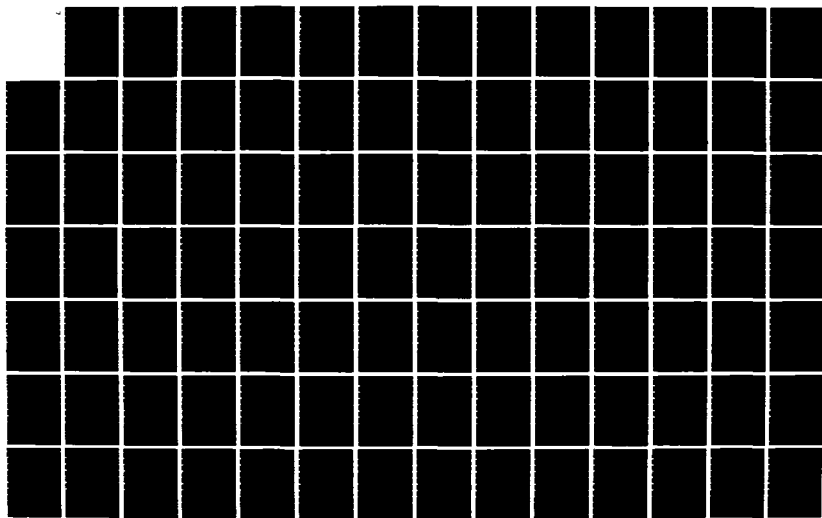
2/3

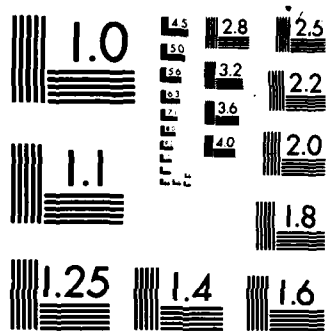
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F/G 9/2

NL





MICROCOPY RESOLUTION TEST CHART  
NATIONAL BUREAU OF STANDARDS 1963-A

```
0001      SUBROUTINE REGAIN(R,S,G,EPS,MR,MF,NCH)
      C      WRITTEN BY G.W. PHILLIPS
      C      NAVAL RESEARCH LABORATORY
      C      LAST REVISED AUGUST 1981 BY G.W.P.
      C
      C      PERFORMS DIGITAL GAIN AND ZERO SHIFT
      C      ON SPECTRAL DATA
      C
0002      DIMENSION R(1),S(1)
      C
      C      THE EFFECT OF THIS SUBROUTINE IS TO FIRST ADJUST THE
      C      GAIN BY G, AND THEN TO SHIFT THE DATA BY EPS
      C
      C      R=INITIAL DATA ARRAY, S=SHIFTED DATA ARRAY
      C      G=GAIN SHIFT, EPS=ZERO SHIFT, MF=OFFSET FOR CHANNEL 1
      C      MR=NUMBER OF DATA CHANNELS, NCH=MAXIMUM NUMBER OF CHANNELS
      C
0003      IF(G.NE.1.0.OR.EPS.NE.0.0) GOTO 100
0005      DO 50 J=1,NCH
0006      50      S(J)=R(J)
0007      RETURN
      C
0008      100  DO 110 J=1,NCH
0009      110      S(J)=0.
0010      MI=MF-1
0011      AT=G*(MR+MI)+EPS
0012      MT=INT(AT)
0013      MT=MIN0(MT,NCH)
0014      MRI=MR
0015      MJ=INT(G*MI+EPS)
0016      MJ=MAX0(MJ,0)
0017      MF=MJ+1
0018      MR=MT-MJ
0019      GINV=1./G
0020      IF(G.GT.1) GO TO 300
```

C

```
C
C
C   DISTRIBUTE COUNTS (REBIN)
C
0022   DO 200 I=1,MRI
0023       A=G*(I+MI)+EPS
0024       IF(A.LT.0) GOTO 200
0026       J=INT(A)
0027       DJ=A-J
0028       J=J-MJ
0029       IF(J.LT.0.OR.J.GT.MR) GOTO 200
0031       IF(DJ.LT.0) GO TO 160
0033       IF(J.LT.MR) S(J+1)=S(J+1)+R(I)
0035       GOTO 200
0036   160   DR=DJ*GINV*R(I)
0037       IF(J.LT.MR) S(J+1)=S(J+1)+DR
0039       IF(J.GT.0) S(J)=S(J)+R(I)-DR
0041   200   CONTINUE
0042       JM=J+1
0043       DJM=DJ
C
C   EXTRAPOLATE ENDS
C
0044       A0=G*MI+EPS
0045       IF(A0.LE.0) GOTO 240
0047       J=INT(A0)
0048       DJ=A0-J
0049       J=J-MJ
0050       IF(J.LT.0) GOTO 240
0052       S(J+1)=S(J+1)+DJ*GINV*R(I)
0053       IF(J.LT.1) GOTO 240
0055       J0=J
0056       DO 220 J=1,J0
0057   220       S(J)=GINV*R(I)
C
0058   240   IF(JM.GT.MR) RETURN
0060       S(JM)=S(JM)+(1-DJM)*GINV*R(MRI)
0061       JM=JM+1
0062       IF(JM.GT.MR) RETURN
0064       DO 260 J=JM,MR
0065   260       S(J)=GINV*R(MRI)
0066       RETURN
```

C  
C  
C  
C

INTERPOLATE BETWEEN MIDPOINTS

```
0067 300 DO 400 J=1,MR
0068      A=FLOAT(J+MJ)-0.5
0069      I=INT((A-EPS)*GINV)
0070      B=G*(I-0.5)+EPS
0071      I=I-MI
0072      IF(A-B.LE.G) GOTO 340
0074      I=I+1
0075      B=B+G
0076 340 IF(I.GT.0) GOTO 350
0078      S(J)=R(I)*GINV
0079      GOTO 400
0080 350 IF(I.LT.MRI) GOTO 360
0082      S(J)=R(MRI)*GINV
0083      GOTO 400
0084 360 DG=(A-B)*GINV
0085      S(J)=DG*R(I+1)*GINV+(1.-DG)*R(I)*GINV
0086 400 CONTINUE
0087      RETURN
0088      END
```

# MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
R	000014	REAL*4 PARAMETER ARRAY (1)
S	000016	REAL*4 PARAMETER ARRAY (1)
G	000020	REAL*4 PARAMETER VARIABLE
EPS	000022	REAL*4 PARAMETER VARIABLE
MR	000024	INTEGER*2 PARAMETER VARIABLE
MF	000026	INTEGER*2 PARAMETER VARIABLE
NCH	000030	INTEGER*2 PARAMETER VARIABLE
J	000034	INTEGER*2 VARIABLE
MI	000036	INTEGER*2 VARIABLE
AT	000040	REAL*4 VARIABLE
MT	000044	INTEGER*2 VARIABLE
INT	000000	INTEGER*2 PROCEDURE
MIN0	000000	INTEGER*2 PROCEDURE
MRI	000046	INTEGER*2 VARIABLE
MJ	000050	INTEGER*2 VARIABLE
MAX0	000000	INTEGER*2 PROCEDURE
GINV	000052	REAL*4 VARIABLE
I	000056	INTEGER*2 VARIABLE
A	000060	REAL*4 VARIABLE
DJ	000064	REAL*4 VARIABLE
DR	000070	REAL*4 VARIABLE
JM	000074	INTEGER*2 VARIABLE
DJM	000076	REAL*4 VARIABLE
AO	000102	REAL*4 VARIABLE
JO	000106	INTEGER*2 VARIABLE
FLOAT	000000	REAL*4 PROCEDURE
B	000110	REAL*4 VARIABLE
DE	000114	REAL*4 VARIABLE

```
0001      SUBROUTINE RECHAN(R,S,MR,MF,NCH)
          C      WRITTEN BY G.W.PHILLIPS, AUGUST 1981
          C
          C      SHIFTS DATA IN ARRAY S BY MF-1 CHANNELS
          C      AND STORES THE SHIFTED DATA IN ARRAY R
0002      DIMENSION R(256),S(256)
          C
0003      100  K=MF-1
0004           MF=1
0005           MR=MR+K
0006           IF(MF.LT.0) MR=0
0008           IF(MR.GT.NCH) MR=NCH
0010           J=1
0011           IF(K.LT.1) GOTO 120
0013           J=K+1
0014           DO 110 I=1,K
0015      110  R(I)=0.
0016      120  DO 130 I=J,MR
0017      130  R(I)=S(I-K)
0018           L=MR+1
0019           IF(L.GT.NCH) RETURN
0021           DO 140 I=L,NCH
0022      140  R(I)=0.
0023           RETURN
0024           END
```

# MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
R	000014	REAL*4 PARAMETER ARRAY (256)
S	000016	REAL*4 PARAMETER ARRAY (256)
MR	000020	INTEGER*2 PARAMETER VARIABLE
MF	000022	INTEGER*2 PARAMETER VARIABLE
NCH	000024	INTEGER*2 PARAMETER VARIABLE
K	000026	INTEGER*2 VARIABLE
J	000030	INTEGER*2 VARIABLE
I	000032	INTEGER*2 VARIABLE
L	000034	INTEGER*2 VARIABLE

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SCHAUMBURG, ILLINOIS 60196

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SEDIT MOD 44-0436-01 10 MAR 77 L.HOLMES  
THIS IS THE PREGA LIBRARY FILE EDITOR  
IT BUILDS A LIST OF THE STANDARD ISOTOPE SPECTRA  
TO BE USED FROM THE DISK

# FILE STRUCTURE

## RECORD : PARAMETER

1	NUMBER OF STANDARDS IN LIBRARY
2	NUMBER OF CHANNELS PER STANDARD
3	NUMBER OF ITERATIONS FOR GAIN THRESHOLD SHIFT
4	BACKGROUND SUBTRACT ?
5	INITIAL CHANNEL FOR COMPUTATION
6	FINAL CHANNEL FOR COMPUTATION
7-39	SPACE RESERVED FOR FILE EXPANSION
40	COUNTING TIME FOR BACKGROUND
41	REJECTION COEFFICIENT.
42-49	ID FOR LIBRARY BACKGROUND
50-64	SPACE RESERVED FOR FILE EXPANSION

65-96,97-128,... LIST OF STANDARDS WITH ASSOCIATED PARAMETERS  
I.E.

## RECORD : PARAMETER

65	EIGHT CHARACTER NAME OF STANDARD
66-73	FILE ELEMENT ID
74	HALF-LIFE
75	COUNTING TIME OF SAMPLE

76 ACTIVITY OF SAMPLE

0001  
0002

INTEGER ANS,YES  
DATA YES,NO/1HY,1HN/

```

0003      INTEGER INT(26),MLI(40)
0004      LOGICAL*1 A(32)
0005      DATA LN/1HN/
0006      DATA LI,LD,LA,LP/1HI,1HD,1HA,1HL/
0007      INTEGER BB,CC
0008      DATA BB,CC/1HB,1HC/
0009      INTEGER BS,BT,RC,BA
0010      DATA NC,IT,BS,IS,IE,LL,LS,BT,RC,BA
1/2HNC,2HIT,2HBS,2HIS,2HIE,2HLL,2HLS,2HBT,2HRC,2HBA/
0011      INTEGER Y,D,H
0012      DATA Y,D,H,MM/1HY,1HD,1HH,1HM/
0013      INTEGER EDT
0014      EDT=0
0015      L=5
0016      N=0
0017      LUN=9
0018      LUI=11
0019      DO 1200 I=1,40
0020 1200    MLI(I)=I
0021      DEFINE FILE LUN(4096,2,U,IVAR)
0022      DEFINE FILE LUI(4096,2,U,IVAR)
0023      IVAR=1
0024      READ(LUN*1,END=500,ERR=600)M
0025      WRITE(5,1)
0026 1      FORMAT(1X,'PREGA LIBRARY FILE EDITOR',/)
0027 10000   CONTINUE
0028 1999   WRITE(5,2000)
0029 2000   FORMAT(1X,'HEADER: BUILD(B), CHANGE(C), LIST(L) ',)
0030      READ(5,5000)LENGTH,ANS
0031      IF(LENGTH.LE.0)GO TO 15
0033      IF(ANS.EQ.BB)GO TO 2001
0035      IF(ANS.EQ.CC)GO TO 2500
0037      IF(ANS.EQ.LP)GO TO 6500
0039      GO TO 10000
0040 2001   ASSIGN 2050 TO K
0041 2040   WRITE(5,2041)
0042 2041   FORMAT(' ',(NC) NUMBER OF CHANNELS PER STANDARD (MAX=512) ',)
0043 2042   READ(5,5001)LENGTH,FNUM
0044      IF(LENGTH.LE.0)GO TO 10000
0046      IF(FNUM.GT.512.)FNUM=512.
0048      IF(FNUM.LE.1.0)FNUM=1.0
0050      NUM=FNUM
0051      WRITE(LUN*2)NUM
0052      GO TO K
0053 2050   ASSIGN 2060 TO K
0054      WRITE(5,2051)
0055 2051   FORMAT(' ',(IT) NUMBER OF ITERATIONS FOR THRESHOLD & GAIN CALC.
1',)
0056 2052   READ(5,5001)LENGTH,FNUM
0057      IF(LENGTH.LE.0)GO TO 10000
0059      IF(FNUM.LE.1.0)FNUM=1.0
0061      NUM=FNUM
0062      WRITE(LUN*3)NUM
0063      GO TO K
0064 2060   ASSIGN 2070 TO K
0065      WRITE(5,2061)
0066 2061   FORMAT(' ',(BS) BACKGROUND SUBTRACT ? ',)

```

```
0067 2062 READ(5,5000)LENGTH,ANS
0068      IF(LENGTH.LE.0)GO TO 10000
0070      NUM=0
0071      IF(ANS.EQ.YES)NUM=1
0073      WRITE(LUN'4)NUM
0074      GO TO K
0075 2070 ASSIGN 2080 TO K
0076      WRITE(5,2071)
0077 2071 FORMAT(' ','(IS) INITIAL CHANNEL FOR COMPUTATION ',%)
0078 2072 READ(5,5001)LENGTH,FNUM
0079      IF(LENGTH.LE.0)GO TO 10000
0081      IF(FNUM.GT.512.)FNUM=512.
0083      IF(FNUM.LE.1.0)FNUM=1.0
0085      NUM=FNUM
0086      WRITE(LUN'5)NUM
0087      GO TO K
0088 2080 ASSIGN 2110 TO K
0089      WRITE(5,2081)
0090 2081 FORMAT(' ','(IE) FINAL CHANNEL FOR COMPUTATION ',%)
0091 2082 READ(5,5001)LENGTH,FNUM
0092      IF(LENGTH.LE.0)GO TO 10000
0094      IF(FNUM.GT.512.)FNUM=512.
0096      IF(FNUM.LE.1.0)FNUM=1.0
0098      NUM=FNUM
0099      WRITE(LUN'6)NUM
0100      GO TO K
0101 2110 ASSIGN 2120 TO K
0102      WRITE(5,2111)
0103 2111 FORMAT(' ','(BT) COUNTING TIME OF BACKGROUND (SECS.) ',%)
0104 2112 READ(5,5001)LENGTH,FNUM
0105      IF(LENGTH.LE.0)GO TO 10000
0107      IF(FNUM.LE.1.0)FNUM=1.0
0109      WRITE(LUN'40)FNUM
0110      GO TO K
0111 2120 ASSIGN 2130 TO K
0112      WRITE(5,2121)
0113 2121 FORMAT(' ','(RC) REJECTION COEFICIENT ',%)
0114 2122 READ(5,5001)LENGTH,FNUM
0115      IF(LENGTH.LE.0)GO TO 10000
0117      WRITE(LUN'41)FNUM
0118      GO TO K
0119 2130 ASSIGN 2140 TO K
0120      WRITE(5,2131)
0121 2131 FORMAT(' ','(BA) BACKGROUND SPECTRUM (FILE.ELEMENT(.DEVICE)) ',/)
0122 2132 READ(5,4)LENGTH,(A(I),I=1,32)
0123      IF(LENGTH.LE.0)GO TO 10000
0125      IVAR=42
0126      DO 2133 I=1,32,4
0127 2133 WRITE(LUN'IVAR)A(I),A(I+1),A(I+2),A(I+3)
0128      GO TO K
0129 2140 GO TO 1999
0130 2500 ASSIGN 2500 TO K
0131      WRITE(5,2501)
0132 2501 FORMAT(' ','WHICH PARAMETER DO YOU WISH TO MODIFY ? ',%)
0133      READ(5,5007)LENGTH,ANS
0134      IF(LENGTH.LE.0)GO TO 10000
0136      IF(ANS.EQ.NC)GO TO 6000
```

```
0138      IF(ANS.EQ.IT)GO TO 6001
0140      IF(ANS.EQ.BS)GO TO 6002
0142      IF(ANS.EQ.IS)GO TO 6003
0144      IF(ANS.EQ.IE)GO TO 6004
0146      IF(ANS.EQ.BT)GO TO 6007
0148      IF(ANS.EQ.RC)GO TO 6008
0150      IF(ANS.EQ.BA)GO TO 6009
0152      GO TO 2500
0153 6000  READ(LUN'2)NUM
0154      WRITE(L,2041)
0155      WRITE(L,5004)NUM
0156      IF(EDT.EQ.1)GO TO 7000
0158      GO TO 2042
0159 6001  READ(LUN'3)NUM
0160      WRITE(L,2051)
0161      WRITE(L,5004)NUM
0162      IF(EDT.EQ.1)GO TO 7000
0164      GO TO 2052
0165 6002  READ(LUN'4)NUM
0166      WRITE(L,2061)
0167      ANS=NO
0168      IF(NUM.EQ.1)ANS=YES
0170      WRITE(L,5008)ANS
0171      IF(EDT.EQ.1)GO TO 7000
0173      GO TO 2062
0174 6003  READ(LUN'5)NUM
0175      WRITE(L,2071)
0176      WRITE(L,5004)NUM
0177      IF(EDT.EQ.1)GO TO 7000
0179      GO TO 2072
0180 6004  READ(LUN'6)NUM
0181      WRITE(L,2081)
0182      WRITE(L,5004)NUM
0183      IF(EDT.EQ.1)GO TO 7000
0185      GO TO 2082
0186 6007  READ(LUN'40)FNUM
0187      WRITE(L,2111)
0188      WRITE(L,5005)FNUM
0189      IF(EDT.EQ.1)GO TO 7000
0191      GO TO 2112
0192 6008  READ(LUN'41)FNUM
0193      WRITE(L,2121)
0194      WRITE(L,5005)FNUM
0195      IF(EDT.EQ.1)GO TO 7000
0197      GO TO 2122
0198 6009  IVAR=42
0199      DO 2600 I=1,32,4
0200 2600  READ(LUN'IVAR)A(I),A(I+1),A(I+2),A(I+3)
0201      WRITE(L,2131)
0202      WRITE(L,5006)(A(I),I=1,32)
0203      IF(EDT.EQ.1)GO TO 7000
0205      GO TO 2132

C  HEADER LISTER
0206 6500  CONTINUE
0207      L=6
0208      EDT=1
0209      WRITE(L,6501)
```

```
0210 6501 FORMAT('1', '          PREGA LIBRARY HEADER', //)
0211      I=0
0212 7000 I=I+1
0213      IF(I.GT. 8)GO TO 6010
0215      GO TO (6000,6001,6002,6003,6004,          6007,6008,6009) ,I
0216 6010 L=5
0217      EDT=0
0218      WRITE(6,411)
0219      WRITE(6,411)
0220      GO TO 1999
0221 3000 CONTINUE
0222 15 CONTINUE
0223      WRITE(5,16)
0224 16 FORMAT(1X,'LIST OF STANDARDS')
0225      WRITE(5,111)
0226 111 FORMAT(1X,'NEW FILE(N),INSERT(I),DELETE(D),APPEND(A),LIST(L) ', $)
0227      IVAR=1
0228      N=0
0229      EDT=0
0230      READ(5,2)LENGTH,ANS
0231 2 FORMAT(Q,A1)
0232      IF(LENGTH.EQ.0)GO TO 1000
0233      IF(ANS.EQ.LN)GO TO 25
0236      IF(ANS.EQ.LI)GO TO 100
0238      IF(ANS.EQ.LD)GO TO 200
0240      IF(ANS.EQ.LA)GO TO 300
0242      IF(ANS.EQ.LP)GO TO 400
0244      GO TO 15
0245 25 CONTINUE
0246      IVAR=65+N*16
0247      WRITE(5,20)
0248 20 FORMAT(1X,'ISOTOPE NAME (8 CHARACTERS MAX) ', $)
0249      READ(5,21)LENGTH,(A(I),I=1,8)
0250 21 FORMAT(Q,8A1)
0251      IF(LENGTH.EQ.0)GO TO 15
0253      DO 22 I=1,8,4
0254 22 WRITE(LUN' IVAR)A(I),A(I+1),A(I+2),A(I+3)
0255      WRITE(5,3)
0256 3 FORMAT(1X,'FILE.ELEMENT(,DEVICE) ', $)
0257      READ(5,4)LENGTH,(A(I),I=1,32)
0258 4 FORMAT(Q,32A1)
0259      IF(LENGTH.EQ.0)GO TO 15
0261      DO 10 I=1,32,4
0262 10 WRITE(LUN' IVAR,END=500,ERR=600)A(I),A(I+1),A(I+2),A(I+3)
0263      WRITE(5,5)
0264 5 FORMAT(1X,'HALF-LIFE,UNITS(Y,D,H,M,S) ', $)
0265      READ(5,6)LENGTH,HL,K
0266 6 FORMAT(Q,E12.0,1A1)
0267      IF(LENGTH.EQ.0)GO TO 15
0269      IF(K.EQ.Y)HL=HL*31536000.
0271      IF(K.EQ.D)HL=HL*86400.
0273      IF(K.EQ.H)HL=HL*3600.
0275      IF(K.EQ.MM)HL=HL*60.
0277      WRITE(LUN' IVAR)HL
0278      WRITE(5,7)
0279 7 FORMAT(1X,'COUNTING TIME OF STANDARD (SECS.) ', $)
0280      READ(5,5001)LENGTH,SEC
```

```
0281      IF(LENGTH.EQ.0)GO TO 15
0283      IF(SEC.LE.1.0)SEC=1.0
0285      WRITE(LUN'IVAR)SEC
0286      WRITE(5,9)
0287  9      FORMAT(1X,'ACTIVITY (MAY BE SET TO 1) ', $)
0288      READ(5,5001)LENGTH,ACT
0289      IF(LENGTH.EQ.0)GO TO 15
0291      WRITE(LUN'IVAR)ACT
0292      IF(EDT.EQ.1)GO TO 15
0294      N=N+1
0295      M=N
0296      WRITE(LUN'1)M
0297      GO TO 25
0298  100     WRITE(5,101)
0299  101     FORMAT(1X,'NUMBER OF ENTRY TO BE INSERTED ', $)
0300      READ(5,102)FNUM
0301  102     FORMAT(F10.0)
0302      NUM=FNUM
0303      N=M
0304      IF(N.LT.NUM)GO TO 15
0306      M=M+1
0307      N=M
0308      EDT=1
0309  103     IF(N.LT.NUM)GO TO 25
0311      IVAR=65+(N-1)*16
0312      DO 104 I=1,26,2
0313  104     READ(LUN'IVAR)INT(I),INT(I+1)
0314      IVAR=IVAR+3
0315      DO 105 I=1,26,2
0316  105     WRITE(LUN'IVAR)INT(I),INT(I+1)
0317      N=N-1
0318      GO TO 103
0319  C
0319  200     WRITE(5,201)
0320  201     FORMAT(1X,'NUMBER OF ENTRY TO BE DELETED ', $)
0321      READ(5,202)FNUM
0322  202     FORMAT(F10.0)
0323      NUM=FNUM
0324      IF(NUM.GT.M)GO TO 15
0326      IF(NUM.EQ.M)GO TO 206
0328      IF(M.LE.0)GO TO 206
0330  203     CONTINUE
0331      IVAR=NUM*16+65
0332      DO 204 I=1,26,2
0333  204     READ(LUN'IVAR,END=500,ERR=600)INT(I),INT(I+1)
0334      IVAR=IVAR-29
0335      DO 205 I=1,26,2
0336  205     WRITE(LUN'IVAR,END=500,ERR=600)INT(I),INT(I+1)
0337      NUM=NUM+1
0338      IF(NUM.LT.M)GO TO 203
0340  206     CONTINUE
0341      M=M-1
0342      GO TO 15
0343  300     N=M
0344      GO TO 25
0345  400     IF(M.EQ.0)GO TO 15
0345  C*****
```

```
0347 1008 WRITE(5,1010)
0348 1010 FORMAT(' ','DO YOU WISH TO PRINT FULL STANDARD LIST?',5)
0349 READ(5,2)LENGTH,ANS
0350 IF(LENGTH.LE.0) GO TO 1008
0352 IF(ANS.EQ.YES)GO TO 1020
0354 READ(LUI'29) MLA
D WRITE(6,7100) MLA
D7100 FORMAT(' ',' MLA=',16)
D WRITE(5,7105)
D7105 FORMAT(' ',' IVAR=?',5)
D READ(5,7106) IVAR
D7106 FORMAT(I2)
0355 IVAR=44
0356 DO 1014 I=1,MLA
0357 READ(LUI'IVAR) MLI(I)
D WRITE(6,7110) IVAR,I,MLI(I)
D7110 FORMAT(' ',' IVAR=',13,' MLI(',12,')=',16)
0358 1014 CONTINUE
0359 WRITE(6,1016)
0360 1016 FORMAT('1', ' PREGA LIBRARY STANDARDS USED',//)
0361 GO TO 1024
0362 1020 MLA=M
D WRITE(6,7120) MLA
D7120 FORMAT(' ',' MLA=M=',14)
0363 WRITE(6,401)
0364 401 FORMAT('1', ' PREGA LIBRARY STANDARDS',//)
0365 1024 DO 1090 JI=1,MLA
0366 IVAR=65+16*(MLI(JI)-1)
0367 DO 415 I=1,8,4
0368 415 READ(LUN'IVAR)A(I),A(I+1),A(I+2),A(I+3)
0369 WRITE(6,425)MLI(JI),(A(I),I=1,8)
0370 425 FORMAT(1X,'STANDARD * ',12,' : ',8A1)
0371 DO 404 I=1,32,4
0372 404 READ(LUN'IVAR)A(I),A(I+1),A(I+2),A(I+3)
0373 WRITE(6,3)
0374 WRITE(6,405)(A(I),I=1,32)
0375 405 FORMAT('+', ' : ',32A1)
0376 READ(LUN'IVAR)SEC
0377 WRITE(6,406)SEC
0378 406 FORMAT(1X,'HALF-LIFE (SECS):',1PE12.4)
0379 READ(LUN'IVAR)HL
0380 WRITE(6,407)HL
0381 407 FORMAT(1X,'COUNTING TIME OF STANDARD (SECS):',1PE12.4)
0382 READ(LUN'IVAR)ACT
0383 WRITE(6,408)ACT
0384 408 FORMAT(1X,'ACTIVITY:',1PE12.4,//)
0385 1090 CONTINUE
C *****
0386 410 WRITE(6,411)
0387 WRITE(6,411)
0388 WRITE(6,411)
0389 WRITE(6,411)
0390 WRITE(6,411)
0391 WRITE(6,411)
0392 WRITE(6,411)
0393 WRITE(6,411)
0394 411 FORMAT('+',
```

```
0395      GO TO 15
0396 500   WRITE(5,501)
0397 501   FORMAT(1X,'FILE NOT LARGE ENOUGH')
0398      GO TO 1000
0399 600   WRITE(5,601)
0400 601   FORMAT(1X,'FILE SET UP NOT CORRECT')
0401      GO TO 1000
0402 5000  FORMAT(Q,A1)
0403 5001  FORMAT(Q,E12.0)
0404 5003  FORMAT(Q,32A1)
0405 5004  FORMAT('+',': ',I4,/)
0406 5005  FORMAT('+',': ',G12.6,/)
0407 5006  FORMAT(1X,'      : ',32A1,/)
0408 5007  FORMAT(Q,A2)
0409 5008  FORMAT('+',': ',1A1,/)
0410 1000  IF(M.GE.40)M=40
0412      WRITE(LUN'1)M
0413      END
```

## MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
INT	000006	INTEGER*2 ARRAY (26)
MLI	000072	INTEGER*2 ARRAY (40)
A	000212	LOGICAL*1 ARRAY (32)
ANS	003000	INTEGER*2 VARIABLE
YES	000252	INTEGER*2 VARIABLE
BB	000270	INTEGER*2 VARIABLE
CC	000272	INTEGER*2 VARIABLE
BS	000300	INTEGER*2 VARIABLE
BT	000312	INTEGER*2 VARIABLE
RC	000314	INTEGER*2 VARIABLE
BA	000316	INTEGER*2 VARIABLE
Y	000320	INTEGER*2 VARIABLE
D	000322	INTEGER*2 VARIABLE
H	000324	INTEGER*2 VARIABLE
EDT	003002	INTEGER*2 VARIABLE
NO	000254	INTEGER*2 VARIABLE
LN	000256	INTEGER*2 VARIABLE
LI	000260	INTEGER*2 VARIABLE
LD	000262	INTEGER*2 VARIABLE
LA	000264	INTEGER*2 VARIABLE
LP	000266	INTEGER*2 VARIABLE
NC	000274	INTEGER*2 VARIABLE
IT	000276	INTEGER*2 VARIABLE
IS	000302	INTEGER*2 VARIABLE
IE	000304	INTEGER*2 VARIABLE
LL	000306	INTEGER*2 VARIABLE
LS	000310	INTEGER*2 VARIABLE
MM	000326	INTEGER*2 VARIABLE
L	003004	INTEGER*2 VARIABLE
N	003006	INTEGER*2 VARIABLE
LUN	003010	INTEGER*2 VARIABLE
LUI	003012	INTEGER*2 VARIABLE
I	003014	INTEGER*2 VARIABLE
IVAR	003016	INTEGER*2 VARIABLE
M	003020	INTEGER*2 VARIABLE
LENGTH	003022	INTEGER*2 VARIABLE
K	003024	INTEGER*2 VARIABLE
FNUM	003026	REAL*4 VARIABLE
NUM	003032	INTEGER*2 VARIABLE
HL	003034	REAL*4 VARIABLE
SEC	003040	REAL*4 VARIABLE
ACT	003044	REAL*4 VARIABLE
MLA	003050	INTEGER*2 VARIABLE
JI	003052	INTEGER*2 VARIABLE

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C  
C UEDIT MOD 44-0435-01 10 MAR 77 L.HOLMES  
C THIS IS THE NAI UNKNOWN LIBRARY EDITOR.  
C IT SETS UP THE ANALYSIS PARAMETERS FOR  
C THE UNKNOWN SAMPLE SPECTRUM.  
C  
C  
C FILE STRUCTURE  
C  
C RECORD : PARAMETER  
C  
C 1-8 ID OF SAMPLE  
C 10 GAIN SHIFT RATIO  
C 11 THRESHOLD SHIFT  
C 12 BACKGROUND SUPPLIED ?  
C 13 BACKGROUND SUBTRACT ?  
C 14 COUNTING TIME FOR BACKGROUND  
C 15 COUNTING TIME FOR UNKNOWN SAMPLE  
C 16 VOLUME REDUCTION FACTOR  
C 17 DECAY TIME  
C 18 RESULT MULTIPLICATION FACTOR  
C 19-27 ID OF SAMPLE BACKGROUND  
C 28 WEIGHTING FACTOR DETERMINATION  
C 29 NUMBER OF STANDARDS USED  
C 30 F-TEST REJECTION COEFFICIENT  
C 31 WEIGHTING FACTOR CALCULATION  
C 32 LIBRARY REJECTION COEFFICIENT APPLIED ?  
C THIS REJECTION COEFFICIENT IS IN SEDIT.  
C 33 BACKGROUND REGRESSION?  
C 34 PIVOT ON BACKGROUND?  
C 35 OUTPUT RESIDUALS?  
C 36-42 ID OF OUTPUT FILE  
C 43,44,... ORDER OF OUTPUT FILE

```
      C
      C
0001      INTEGER CC
0002      INTEGER EDT
0003      INTEGER UN,OP,CB,BG,BS,BT,UT,VR,DT,MF,SB,WD,NS,F0,WF,RC,BR,BP,ANS,
1YES,CRT,RO,RS
0004      DATA UN,OP,CB,BG,BS,BT,VR,DT,MF,SB,WD,NS,F0,WF,RC,BR,BP,RO,RS
1/2HUN,2HOP,2HCB,2HBG,2HBS,2HBT,2HVR,2HDT,2HMF,2HSB,2HWD,2HNS,2HF0,
22HWF,2HRC,2HBR,2HBP,2HRO,2HRS/
0005      INTEGER GN,TH
0006      DATA GN,TH/2HGN,2HTH/
0007      INTEGER OR
0008      DATA OR/2HOR/
0009      DATA UT/2HUT/
0010      DATA NN,CC,LL,YES,NO/1HN,1HC,1HL,1HY,1HN/
0011      INTEGER CT
0012      DATA CT/2HCT/
0013      INTEGER BA
0014      DATA BA/2HBA/
0015      LOGICAL*1 A(32)
0016      LUN=11
0017      DEFINE FILE LUN(4096,2,U,IVAR)
0018      CRT=5
0019      READ(LUN*1)M
0020      WRITE(CRT,1)
0021      1      FORMAT(1X,'PREGA UNKNOWN FILE EDITOR',//)
0022      10000 CONTINUE
0023      1500  WRITE(5,4)
0024      4      FORMAT(1X,'NEW FILE(N), CHANGE(C), LIST(L) ',5)
0025      READ(CRT,1002)LENGTH,ANS
0026      IF(LENGTH.LE.0)GO TO 11000
0028      IVAR=2
0029      IF(ANS.EQ.CC)GO TO 450
0031      IF(ANS.EQ.LL)GO TO 900
0033      IF(ANS.EQ.NN)GO TO 49
0035      GO TO 1500
```

```
C
C BUILD INDIVIDUAL FILES
0036 49  CONTINUE
0037      ASSIGN 60 TO K
0038 50  WRITE(CRT,51)
0039 51  FORMAT(1X,'(UN) UNKNOWN SPECTRUM: FILE.ELEMENT(,DEVICE) ',/)
0040 52  READ(CRT,1001)LENGTH,(A(I),I=1,32)
0041      IF(LENGTH.LE.0)GO TO 10000
0043      DO 55 I=1,32,4
0044 55  WRITE(LUN'IVAR)A(I),A(I+1),A(I+2),A(I+3)
0045      GO TO K
0046 60  ASSIGN 70 TO K
0047      WRITE(CRT,61)
0048 61  FORMAT(1X,'(GN) GAIN SHIFT RATIO ',)
0049 62  READ(CRT,1003)LENGTH,FNUM
0050      IF(LENGTH.LE.0)GO TO 10000
0052      IF(FNUM.LE.(1.0E-5))FNUM=1.0
0054      WRITE(LUN'IVAR)FNUM
0055      GO TO K
0056 70  ASSIGN 80 TO K
0057      WRITE(CRT,71)
0058 71  FORMAT(1X,'(TH) THRESHOLD SHIFT ',)
0059 72  READ(CRT,1003)LENGTH,FNUM
0060      IF(LENGTH.LE.0)GO TO 10000
0062      WRITE(LUN'IVAR)FNUM
0063      GO TO K
0064 80  ASSIGN 90 TO K
0065      WRITE(CRT,81)
0066 81  FORMAT(1X,'(BG) BACKGROUND SUPPLIED ? ',)
0067 82  READ(CRT,1002)LENGTH,ANS
0068      IF(LENGTH.LE.0)GO TO 10000
0070      NUM=0
0071      IF(ANS.EQ.YES)NUM=1
0073      WRITE(LUN'IVAR)NUM
0074      GO TO K
0075 90  ASSIGN 100 TO K
0076      WRITE(CRT,91)
0077 91  FORMAT(1X,'(BS) SUBTRACT BACKGROUND ? ',)
0078 92  READ(CRT,1002)LENGTH,ANS
0079      IF(LENGTH.LE.0)GO TO 10000
0081      NUM=0
0082      IF(ANS.EQ.YES)NUM=1
0084      WRITE(LUN'IVAR)NUM
0085      GO TO K
```

```
C
0086 100  ASSIGN 110 TO K
0087      WRITE(CRT,101)
0088 101  FORMAT(1X,'(BT) COUNTING TIME FOR BACKGROUND (SECS) ',,$)
0089 102  READ(CRT,1003) LENGTH,FNUM
0090      IF(LENGTH.LE.0)GO TO 10000
0092      IF(FNUM.LE.1.0)FNUM=1.0
0094      WRITE(LUN'IVAR)FNUM
0095      GO TO K
0096 110  ASSIGN 120 TO K
0097      WRITE(CRT,111)
0098 111  FORMAT(1X,'(CT) COUNTING TIME FOR UNKNOWN SAMPLE ',,$)
0099 112  READ(CRT,1003)LENGTH,FNUM
0100      IF(LENGTH.LE.0)GO TO 10000
0102      IF(FNUM.LE.1.0)FNUM=1.0
0104      WRITE(LUN'IVAR)FNUM
0105      GO TO K
0106 120  ASSIGN 130 TO K
0107      WRITE(CRT,121)
0108 121  FORMAT(1X,'(VR) VOLUME REDUCTION (OR INVERSE OF DILUTION)',/,1X,
1'      FACTOR ',,$)
0109 122  READ(CRT,1003)LENGTH,FNUM
0110      IF(LENGTH.LE.0)GO TO 10000
0112      IF(FNUM.LE.(1.0E-5))FNUM=1.0
0114      WRITE(LUN'IVAR)FNUM
0115      GO TO K
0116 130  ASSIGN 140 TO K
0117      WRITE(CRT,131)
0118 131  FORMAT(1X,'(DT) DECAY TIME ',,$)
0119 132  READ(CRT,1003)LENGTH,FNUM
0120      IF(LENGTH.LE.0)GO TO 10000
0122      WRITE(LUN'IVAR)FNUM
0123      GO TO K
0124 140  ASSIGN 150 TO K
0125      WRITE(CRT,141)
0126 141  FORMAT(1X,'(MF) RESULT MULTIPLICATION FACTOR ',,$)
0127 142  READ(CRT,1003)LENGTH,FNUM
0128      IF(LENGTH.LE.0)GO TO 10000
0130      WRITE(LUN'IVAR)FNUM
0131      GO TO K
0132 150  ASSIGN 180 TO K
0133      WRITE(CRT,151)
0134 151  FORMAT(1X,'(BA) BACKGROUND SPECTRUM: FILE.ELEMENT(,DEVICE) ',/,)
0135 152  READ(CRT,1001)LENGTH,(A(I),I=1,32)
0136      IF(LENGTH.LE.0)GO TO 10000
0138      DO 153 I=1,32,4
0139 153  WRITE(LUN'IVAR)A(I),A(I+1),A(I+2),A(I+3)
0140      GO TO K
```

```
C
0141 160 ASSIGN 170 TO K
0142 162 WRITE(CRT,161)
0143 161 FORMAT(1X,'ANALYSIS OPTIONS ')
0144      GO TO K
0145 170 ASSIGN 180 TO K
0146      WRITE(CRT,171)
0147 171 FORMAT(1X,'(SB) SUBTRACT BACKGROUND ? ',/$)
0148 172 READ(CRT,1002)LENGTH,ANS
0149      IF(LENGTH.LE.0)GO TO 10000
0151      WRITE(LUN'IVAR)ANS
0152      GO TO K
0153 180 ASSIGN 190 TO K
0154      IVAR=IVAR+1
0155      WRITE(CRT,181)
0156 181 FORMAT(1X,'(WD) HOW ARE WEIGHTING FACTORS TO BE DETERMINED ?',/,1X
      1,
      2'      0: BASED ON ACTUAL COUNTS/CHANNEL.',/,1X,
      3'      1: BASED ON CALCULATED COUNTS/CHN ',/$)
0157 182 READ(CRT,1003)LENGTH,FNUM
0158      IF(LENGTH.LE.0)GO TO 10000
0160      NUM=0
0161      IF(FNUM.EQ.1.0)NUM=1
0163      WRITE(LUN'IVAR)NUM
0164      GO TO K
0165 190 ASSIGN 200 TO K
0166      WRITE(CRT,191)
0167 191 FORMAT(1X,'(NS) NUMBER OF ISOTOPES USED FROM THE STANDARD LIBRARY
      1?'$)
0168 192 READ(CRT,1003)LENGTH,FNUM
0169      IF(LENGTH.LE.0)GO TO 10000
0171      NUM=FNUM
0172      IF(NUM.GE.15)NUM=15
0174      IF(NUM.LE.1)NUM=1
0176      WRITE(LUN'IVAR)NUM
0177      GO TO K
```

```
C
0178 200  ASSIGN 210 TO K
0179      WRITE(CRT,201)
0180 201  FORMAT(1X,'(F0) F-TEST REJECTION COEFFICIENT.', '$)
0181 202  READ(CRT,1003)LENGTH,FNUM
0182      IF(LENGTH.LE.0)GO TO 10000
0184      WRITE(LUN'IVAR)FNUM
0185      GO TO K
0186 210  ASSIGN 220 TO K
0187      WRITE(CRT,211)
0188 211  FORMAT(1X,'(WF) WEIGHTING FACTOR CALCULATION.'
           1,/,1X,'      -1: (COUNTS)**-1 '
           2,/,1X,'      0: (SIGMA)**-2 '
           3,/,1X,'      1: 1 ', '$)
0189 212  READ(CRT,1003)LENGTH,FNUM
0190      IF(LENGTH.LE.0)GO TO 10000
0192      NUM=1
0193      IF(FNUM.EQ.0.0)NUM=0
0195      IF(FNUM.EQ.(-1.0))NUM=-1
0197      NUM=FNUM
0198      WRITE(LUN'IVAR)NUM
0199      GO TO K
0200 220  ASSIGN 230 TO K
0201      WRITE(CRT,221)
0202 221  FORMAT(1X,'(RC) REJECTION COEFFICIENT APPLIED ? ', '$)
0203 222  READ(CRT,1002)LENGTH,ANS
0204      IF(LENGTH.LE.0)GO TO 10000
0206      NUM=0
0207      IF(ANS.EQ.YES)NUM=1
0209      WRITE(LUN'IVAR)NUM
0210      GO TO K
0211 230  ASSIGN 240 TO K
0212      WRITE(CRT,231)
0213 231  FORMAT(1X,'(BR) BACKGROUND REGRESSION ?'
           1,/,6X,' 0: TRIAL SET = CHOSEN STANDARDS'
           2,/,6X,' 1: TRIAL SET = BACKGROUND ONLY', '$)
0214 232  READ(CRT,1003)LENGTH,FNUM
0215      IF(LENGTH.LE.0)GO TO 10000
0217      NUM=FNUM
0218      WRITE(LUN'IVAR)NUM
0219      GO TO K
```

```
      C
0220 240  ASSIGN 243 TO K
0221      WRITE(CRT,241)
0222 241  FORMAT(1X,'(BP) PIVOT ON BACKGROUND SPECTRUM ALLOWED?'
      1,/,6X,' 0: NO PIVOT ON BACKGROUND ALLOWED'
      2,/,6X,' 1: ALLOW PIVOT ON BACKGROUND SPECTRUM',%)
0223 242  READ(CRT,1003)LENGTH,FNUM
0224      IF(LENGTH.LE.0)GO TO 10000
0226      NUM=FNUM
0227      WRITE(LUN'IVAR)NUM
0228      GO TO K
0229 243  ASSIGN 246 TO K
0230      WRITE(CRT,244)
0231 244  FORMAT(1X,'(RO) OUTPUT RESIDUALS ?',%)
0232 245  READ(CRT,1002)LENGTH,ANS
0233      IF(LENGTH.LE.0) GOTO 10000
0235      NUM=0
0236      IF(ANS.EQ.YES) NUM=1
0238      WRITE(LUN'IVAR)NUM
0239      GOTO K
0240 246  ASSIGN 250 TO K
0241      WRITE(CRT,247)
0242 247  FORMAT(1X,'(RS) RESIDUAL SPECTRUM: FILE.ELEMENT(,DEVICE)')
0243 248  READ(CRT,1001)LENGTH,(A(I),I=1,32)
0244      IF(LENGTH.LE.0) GOTO 10000
0246      DO 249 I=1,32,4
0247 249  WRITE(LUN'IVAR)A(I),A(I+1),A(I+2),A(I+3)
0248      GOTO K
0249 250  ASSIGN 10000 TO K
0250      IVAR=IVAR-6
0251      READ(LUN'IVAR)NUM
0252      ITT=NUM
0253      IVAR=IVAR+5
0254      WRITE(CRT,251)
0255 251  FORMAT(1X,'(OR) NUMBER OF LIBRARY STANDARD IN ORDER OF DESIRED ',
      1'PRINTOUT ')
0256 252  DO 253 I=1,ITT
0257      WRITE(CRT,254)
0258 254  FORMAT(1X,'          STANDARD NUMBER : ',%)
0259      READ(CRT,1003)LENGTH,FNUM
0260      IF(LENGTH.LE.0)GO TO 10000
0262      NUM=FNUM
0263      WRITE(LUN'IVAR)NUM
0264 253  CONTINUE
0265      GO TO K
0266 450  IVAR=1
0267      IVAR=2
0268      ASSIGN 450 TO K
```

```
C
C THIS SECTION ENABLES MODIFICATION OF AN EXISTING FILE
0269 500 WRITE(CRT,501)
0270 501 FORMAT(1X,'WHICH PARAMETER DO YOU WISH TO MODIFY ? ',5)
0271 READ(CRT,1000)LENGTH,ANS
0272 IF(LENGTH.LE.0)GO TO 10000
0274 IF(ANS.EQ.UN)GO TO 600
0276 IF(ANS.EQ.GN)GO TO 610
0278 IF(ANS.EQ.TH)GO TO 620
0280 IF(ANS.EQ.BG)GO TO 630
0282 IF(ANS.EQ.BS)GO TO 640
0284 IF(ANS.EQ.BT)GO TO 650
0286 IF(ANS.EQ.CT)GO TO 660
0288 IF(ANS.EQ.VR)GO TO 670
0290 IF(ANS.EQ.DT)GO TO 680
0292 IF(ANS.EQ.MF)GO TO 690
0294 IF(ANS.EQ.BA)GO TO 700
0296 IF(ANS.EQ.WD)GO TO 720
0298 IF(ANS.EQ.NS)GO TO 730
0300 IF(ANS.EQ.F0)GO TO 740
0302 IF(ANS.EQ.WF)GO TO 750
0304 IF(ANS.EQ.RC)GO TO 760
0306 IF(ANS.EQ.BR)GO TO 770
0308 IF(ANS.EQ.BP)GO TO 780
0310 IF(ANS.EQ.RO)GOTO 782
0312 IF(ANS.EQ.RS)GOTO 784
0314 IF(ANS.EQ.OR)GO TO 790
0316 GO TO 500
0317 600 DO 601 I=1,32,4
0318 601 READ(LUN'IVAR)A(I),A(I+1),A(I+2),A(I+3)
0319 WRITE(CRT,51)
0320 WRITE(CRT,1004)(A(I),I=1,32)
0321 IF(EDT.EQ.1)GO TO 2000
0323 IVAR=IVAR-8
0324 GO TO 52
0325 610 IVAR=IVAR+8
0326 READ(LUN'IVAR)FNUM
0327 WRITE(CRT,61)
0328 WRITE(CRT,1007)FNUM
0329 IF(EDT.EQ.1)GO TO 2000
0331 IVAR=IVAR-1
0332 GO TO 62
```

```
C
0333 620  IVAR=IVAR+9
0334      READ(LUN'IVAR)FNUM
0335      WRITE(CRT,71)
0336      WRITE(CRT,1007)FNUM
0337      IF(EDT.EQ.1)GO TO 2000
0339      IVAR=IVAR-1
0340      GO TO 72
0341 630  IVAR=IVAR+10
0342      READ(LUN'IVAR)NUM
0343      WRITE(CRT,81)
0344      ANS=NO
0345      IF(NUM.EQ.1)ANS=YES
0347      WRITE(CRT,1006)ANS
0348      IF(EDT.EQ.1)GO TO 2000
0350      IVAR=IVAR-1
0351      GO TO 82
0352 640  IVAR=IVAR+11
0353      READ(LUN'IVAR)NUM
0354      WRITE(CRT,91)
0355      ANS=NO
0356      IF(NUM.EQ.1)ANS=YES
0358      WRITE(CRT,1006)ANS
0359      IF(EDT.EQ.1)GO TO 2000
0361      IVAR=IVAR-1
0362      GO TO 92
0363 650  IVAR=IVAR+12
0364      READ(LUN'IVAR)FNUM
0365      WRITE(CRT,101)
0366      WRITE(CRT,1007)FNUM
0367      IF(EDT.EQ.1)GO TO 2000
0369      IVAR=IVAR-1
0370      GO TO 102
0371 660  IVAR=IVAR+13
0372      READ(LUN'IVAR)FNUM
0373      WRITE(CRT,111)
0374      WRITE(CRT,1007)FNUM
0375      IF(EDT.EQ.1)GO TO 2000
0377      IVAR=IVAR-1
0378      GO TO 112
0379 670  IVAR=IVAR+14
0380      READ(LUN'IVAR)FNUM
0381      WRITE(CRT,121)
0382      WRITE(CRT,1007)FNUM
0383      IF(EDT.EQ.1)GO TO 2000
0385      IVAR=IVAR-1
0386      GO TO 122
```

```
C
0387 680  IVAR=IVAR+15
0388      READ(LUN'IVAR)FNUM
0389      WRITE(CRT,131)
0390      WRITE(CRT,1007)FNUM
0391      IF(EDT.EQ.1)GO TO 2000
0393      IVAR=IVAR-1
0394      GO TO 132
0395 690  IVAR=IVAR+16
0396      READ(LUN'IVAR)FNUM
0397      WRITE(CRT,141)
0398      WRITE(CRT,1007)FNUM
0399      IF(EDT.EQ.1)GO TO 2000
0401      IVAR=IVAR-1
0402      GO TO 142
0403 700  IVAR=IVAR+17
0404      DO 701 I=1,32,4
0405 701  READ(LUN'IVAR)A(I),A(I+1),A(I+2),A(I+3)
0406      WRITE(CRT,151)
0407      WRITE(CRT,1004)(A(I),I=1,32)
0408      IF(EDT.EQ.1)GO TO 2000
0410      IVAR=IVAR-8
0411      GO TO 152
0412 710  IVAR=IVAR+25
0413      READ(LUN'IVAR)NUM
0414      WRITE(CRT,171)
0415      ANS=NO
0416      IF(NUM.EQ.1)ANS=YES
0418      WRITE(CRT,1006)ANS
0419      IF(EDT.EQ.1)GO TO 2000
0421      IVAR=IVAR-1
0422      GO TO 172
0423 720  IVAR=IVAR+26
0424      READ(LUN'IVAR)NUM
0425      WRITE(CRT,181)
0426      WRITE(CRT,1005)NUM
0427      IF(EDT.EQ.1)GO TO 2000
0429      IVAR=IVAR-1
0430      GO TO 182
0431 730  IVAR=IVAR+27
0432      READ(LUN'IVAR)NUM
0433      WRITE(CRT,191)
0434      WRITE(CRT,1005)NUM
0435      IF(EDT.EQ.1)GO TO 2000
0437      IVAR=IVAR-1
0438      GO TO 192
```

```
      C
0439 740  IVAR=IVAR+28
0440      READ(LUN,IVAR)FNUM
0441      WRITE(CRT,201)
0442      WRITE(CRT,1007)FNUM
0443      IF(EDT.EQ.1)GO TO 2000
0445      IVAR=IVAR-1
0446      GO TO 202
0447 750  IVAR=IVAR+29
0448      READ(LUN,IVAR)NUM
0449      WRITE(CRT,211)
0450      WRITE(CRT,1005)NUM
0451      IF(EDT.EQ.1)GO TO 2000
0453      IVAR=IVAR-1
0454      GO TO 212
0455 760  IVAR=IVAR+30
0456      READ(LUN,IVAR)NUM
0457      WRITE(CRT,221)
0458      ANS=NO
0459      IF(NUM.EQ.1)ANS=YES
0461      WRITE(CRT,1006)ANS
0462      IF(EDT.EQ.1)GO TO 2000
0464      IVAR=IVAR-1
0465      GO TO 222
0466 770  IVAR=IVAR+31
0467      READ(LUN,IVAR)NUM
0468      WRITE(CRT,231)
0469      WRITE(CRT,1005)NUM
0470      IF(EDT.EQ.1)GO TO 2000
0472      IVAR=IVAR-1
0473      GO TO 232
0474 780  IVAR=IVAR+32
0475      READ(LUN,IVAR)NUM
0476      WRITE(CRT,241)
0477      WRITE(CRT,1005)NUM
0478      IF(EDT.EQ.1)GO TO 2000
0480      IVAR=IVAR-1
0481      GO TO 242
```

```
C
0482 782  IVAR=IVAR+33
0483      READ(LUN' IVAR)NUM
0484      WRITE(CRT,244)
0485      ANS=NO
0486      IF(NUM.EQ.1) ANS=YES
0488      WRITE(CRT,1006)ANS
0489      IF(EDT.EQ.1) GOTO 2000
0491      IVAR=IVAR-1
0492      GOTO 245
0493 784  IVAR=IVAR+34
0494      DO 785 I=1,32,4
0495 785  READ(LUN' IVAR)A(I),A(I+1),A(I+2),A(I+3)
0496      WRITE(CRT,247)
0497      WRITE(CRT,1004)(A(I),I=1,32)
0498      IF(EDT.EQ.1) GOTO 2000
0500      IVAR=IVAR-8
0501      GOTO 248
0502 790  IVAR=IVAR+27
0503      READ(LUN' IVAR)NUM1
0504      ITT=NUM1
0505      WRITE(CRT,251)
0506      IVAR=IVAR+14
0507 796  WRITE(CRT,792)
0508 792  FORMAT(1X,'      : ', $)
0509 795  DO 793 I=1,ITT
0510      READ(LUN' IVAR)NUM
0511      WRITE(CRT,794)NUM
0512 794  FORMAT('+',I3,$)
0513      IF(I.LT.18)GO TO 793
0515      IF(ITT.EQ.18)GO TO 793
0517      ITT=ITT-18
0518      GO TO 796
0519 793  CONTINUE
0520      IF(EDT.EQ.1)GO TO 2000
0522      ITT=NUM1
0523      IVAR=IVAR-NUM1
0524      WRITE(CRT,797)
0525 797  FORMAT(' ')
0526      GO TO 252
```

```
C
0527 900  CONTINUE
0528      CRT=6
0529      EDT=1
0530      WRITE(CRT,901)
0531 901  FORMAT('1','      PREGA UNKNOWN SAMPLE PARAMETERS',//)
0532      II=0
0533 2000  II=II+1
0534      IVAR=2
0535      IF(II.GT.21)GO TO 2001
0537      GO TO (600,610,620,630,640,650,660,670,680,690,700,720,730,740
1,750,760,770,780,782,784,790) II
0538 2001  CONTINUE
0539      EDT=0
0540      WRITE(CRT,1009)
0541      WRITE(CRT,1008)
0542      WRITE(CRT,1008)
0543      WRITE(CRT,1008)
0544      WRITE(CRT,1008)
0545      WRITE(CRT,1008)
0546      WRITE(CRT,1008)
0547      WRITE(CRT,1008)
0548      CRT=5
0549      GO TO 1500
0550 1000  FORMAT(Q,A2)
0551 1001  FORMAT(Q,32A1)
0552 1002  FORMAT(Q,1A1)
0553 1003  FORMAT(Q,E12.0)
0554 1004  FORMAT(1X,'      : ',32A1,/)
0555 1005  FORMAT('+' ,': ',15,/)
0556 1006  FORMAT('+' ,': ',1A1,/)
0557 1007  FORMAT('+' ,': ',G14.6,/)
0558 1008  FORMAT('+' ,')
0559 1009  FORMAT(' ')
0560 11000 CONTINUE
0561      END
```

## MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
A	000006	LOGICAL*1 ARRAY (32)
CC	000126	INTEGER*2 VARIABLE
EDT	003236	INTEGER*2 VARIABLE
UN	000046	INTEGER*2 VARIABLE
OP	000050	INTEGER*2 VARIABLE
CB	000052	INTEGER*2 VARIABLE
BG	000054	INTEGER*2 VARIABLE
BS	000056	INTEGER*2 VARIABLE
BT	000060	INTEGER*2 VARIABLE
UT	000122	INTEGER*2 VARIABLE
VR	000062	INTEGER*2 VARIABLE
DT	000064	INTEGER*2 VARIABLE
MF	000066	INTEGER*2 VARIABLE
SB	000070	INTEGER*2 VARIABLE
WD	000072	INTEGER*2 VARIABLE
NS	000074	INTEGER*2 VARIABLE
F0	000076	INTEGER*2 VARIABLE
WF	000100	INTEGER*2 VARIABLE
RC	000102	INTEGER*2 VARIABLE
BR	000104	INTEGER*2 VARIABLE
BP	000106	INTEGER*2 VARIABLE
ANS	003240	INTEGER*2 VARIABLE
YES	000132	INTEGER*2 VARIABLE
CRT	003242	INTEGER*2 VARIABLE
RO	000110	INTEGER*2 VARIABLE
RS	000112	INTEGER*2 VARIABLE
GN	000114	INTEGER*2 VARIABLE
TH	000116	INTEGER*2 VARIABLE
OR	000120	INTEGER*2 VARIABLE
CT	000136	INTEGER*2 VARIABLE
BA	000140	INTEGER*2 VARIABLE
NN	000124	INTEGER*2 VARIABLE
LL	000130	INTEGER*2 VARIABLE
NO	000134	INTEGER*2 VARIABLE
LUN	003244	INTEGER*2 VARIABLE
IVAR	003246	INTEGER*2 VARIABLE
M	003250	INTEGER*2 VARIABLE
LENGTH	003252	INTEGER*2 VARIABLE
K	003254	INTEGER*2 VARIABLE
I	003256	INTEGER*2 VARIABLE
FNUM	003260	REAL*4 VARIABLE
NUM	003264	INTEGER*2 VARIABLE
ITT	003266	INTEGER*2 VARIABLE
NUM1	003270	INTEGER*2 VARIABLE
II	003272	INTEGER*2 VARIABLE

NAI MOD 44-0434-02 FLPY M12 31 AUG 77 L. HOLMES(SB)  
MODIFIED 5 JUN 81 BY G. PHILLIPS, NRL

MODIFIED TO "PREGA" JULY 82 BY B. G. GLAGOLA, NRL

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PERMISSION OF NUCLEAR DATA.

PURPOSE OF THE PROGRAM:

THIS PROGRAM DETERMINES THE ACTIVITY OF EACH NUCLIDE IN A SPECTRUM  
CONTAINING SEVERAL NUCLIDES WHOSE IDENTITIES ARE KNOWN BUT WHOSE  
ACTIVITIES ARE UNKNOWN. THE PROGRAM ASSUMES SPECTRAL DATA HAS  
BEEN ACQUIRED VIA A SODIUM IODIDE DETECTOR.

METHOD:

THE PROGRAM MAKES A CHANNEL BY CHANNEL COMPARISON BETWEEN THE  
UNKNOWN SPECTRUM AND A SERIES OF STANDARD SPECTRA. IT DETERMINES  
ACTIVITIES BY LEAST SQUARES RESOLUTION OF THE SAMPLE DATA AND  
USES PIVOTAL REGRESSION ANALYSIS TECHNIQUES TO CALCULATE AND  
LIST THE ACTIVITY OF EACH NUCLIDE WITH ESTIMATED ERROR  
AND OTHER INFORMATION ABOUT THE ANALYSIS.

```
C
C
C      VARIABLE DEFINITIONS
C
C      GENERAL CONTROL PARAMETERS
C      (USER DEFINED)
C      NS      = NUMBER OF ISOTOPES IN STANDARD LIBRARY (MAX=80)
C      M       = NUMBER OF CHANNELS PER STANDARD (MAX=512)
C      NIT     = NUMBER OF ITERATION FOR THRESHOLD & GAIN CALC.
C      NBA     = BACKGROUND SUBTRACT (1=YES,0=NO)
C      NZ      = INITIAL CHANNEL FOR COMPUTATION
C      MF      = FINAL CHANNEL FOR COMPUTATION
C      TB      = COUNTING TIME FOR BACKGROUND
C      Q       = REJECTION COEFFICIENT
C      ASC(I)  = STANDARD BACKGROUND SPECTRUM (FILE.ELEMENT(,DEVICE))
C
C
C
C
C
C
C
C
C      CONTROL PARAMETERS FOR EACH LIBRARY ELEMENT
C
C      TISOT(JJ) = ISOTOPE NAME (8 CHARACTERS MAX)
C      HA(I)     = HALF-LIFE (SECS.)
C      TST(I)    = COUNTINUE TIME OF STANDARD
C      AC(I)     = ACTIVITY
C      ASC(I)    = STANDARD SPECTRUM (FILE.ELEMENT(,DEVICE))
C
C
C
```

```
C
C
C CONTROL PARAMETERS FOR UNKNOWN SAMPLE
C (USER DEFINED)
C NBR      = BACKGROUND SUPPLIED ? (YES=1,NO=0)
C NBS      = BACKGROUND SUBTRACT ? (YES=1,NO=0)
C TB       = COUNTING TIME FOR BACKGROUND (SECS)
C TSA      = COUNTING TIME FOR UNKNOWN SAMPLE (SECS)
C VRED     = VOLUME REDUCTION FACTOR (INVERSE OF DILUTION FACTOR)
C DAY      = DECAY TIME (SECS)
C VM       = RESULT MULTIPLICATION FACTOR
C ASC(JJ)  = SAMPLE & BACKGROUND SPECTRUM (FILE.ELEMENT(,DEVICE))
C
C
C
C
C UNKNOWN SAMPLE OPTION VARIABLES
C (USER DEFINED)
C NW       = WEIGHTING FACTOR DETERMINATION (BASED ON ACTUAL
C           COUNTS/CHANNEL=0, BASED ON CALCULATED COUNTS/CHN=1)
C N        = NUMBER OF LIBRARY SPECTRA TO BE FITTED TO SAMPLE
C F0       = F-TEST REJECTION COEFFICIENT
C LW       = WEIGHTING FACTOR CALCULATION ((COUNTS)**-1=-1,
C           (SIGMA)**-2=0, 1=1)
C NEWST    = APPLY REJECTION COEFFICIENT ? (YES=1,NO=0)
C BR       = BACKGROUND REGRESSION (TRIAL SET, CHOSEN STANDARDS=0,
C           BACKGROUND ONLY=1)
C BP       = PIVOT ON BACKGROUND ALLOWED ? (0=NO,1=YES)
C IS(1)    = NUMBER OF LIBRARY STANDARD USED DURING BUILDUP REGRESSION
C ISL(1)   = NUMBER OF LIBRARY STANDARD TO BE FIT IN ORDER OF
C           DESIRED PRINTOUT
C
```

C

```
0001 COMMON/X/FUD
0002 DIMENSION A(10,10),Y(513),Z(10),S(512),STD(10),B(10),
1 R(512),W(512),IR(512),MY(10),FPM(10),FP(10),
2 BA(512),SS(10),AC(10),HA(10),IS(10),TST(10),HAT(10),
3 TNAME(36),TISOT(40),TISO(20),IT(10),SNAM(2),
4F R(10,64),HH(6),SIR(50),ISL(10),HF(4),
SIFORN(20),IFORKL(30),CC(10,10)
0003 DOUBLE PRECISION HG,HR,HT,HF
0004 DATA HF/8HFULL SET,8HTEST SET,8HBACKWARD,8HFORWARD /
0005 DATA HG/8HREGRESN./,HR/8HRESIDUAL/,HT/8HTOTAL /
0006 DATA HH/4HSOUR,4HCE ,4H DF,4H SS,4H MS,4H F /
0007 EQUIVALENCE (BA,IR),(ARR,S),(TNAME(7),SNAM(1))
0008 LOGICAL*1 ASC(60),DEF(10),EF(10)
0009 LOGICAL*1 TNAME
0010 REAL TISO
0011 INTEGER C,D,E,F,MY,P,BR,BP
0012 DATA E/0/
0013 DATA MY/1,2,4,8,16,32,64,128,256,512/
0014 DATA DEF/1HD,1HE,1HF,1H ,1H ,1H8,1H,,1H ,1H ,1H /
0015 DATA TIS1/4HSAMP/,TIS2/4HLE /
0016 DEF(9)=.FALSE.
0017 DEF(10)=.FALSE.
0018 ASC(33)=.FALSE.
0019 ASC(34)=.FALSE.
0020 INTEGER FILE
0021 FILE=8
```

C

C

```
0022 DEFINE FILE 9(4096,2,U,IDAT)
0023 DEFINE FILE 11(4096,2,U,IDAT)
0024 DEFINE FILE 10(0,2,U,IVAR)
```

```
0025      MI=9
0026      MIU=11
0027      MO=6
0028      WRITE(MO,900)
0029      900 FORMAT('1','      OUTPUT FOR PREGA ANALYSIS PROGRAM',////)
C      CHANGE RANGE OF NEXT DO LOOP TO MAX NR OF CHANNELS
0030      DO 1 I=1,512
0031      1 BA(I)=0.0
0032      NNN=0
0033      IPO=0
C
C      GENERAL CONTROL PARAMETERS
C
0034      2 READ(MI'1)NS
0035      READ(MI'2)M
0036      READ(MI'3)NIT
0037      READ(MI'4)NBA
0038      READ(MI'5)NZ
0039      READ(MI'6)MF
0040      READ(MI'40)TB
0041      READ(MI'41)Q
0042      NCH=MF-NZ+1
C
C      (USER DEFINED)
C      NS      = NUMBER OF ISOTOPES IN STANDARD LIBRARY (MAX=80)
C      M       = NUMBER OF CHANNELS PER STANDARD (MAX=512)
C      NIT     = NUMBER OF ITERATION FOR THRESHOLD & GAIN CALC.
C      NIT IS TO BE REMOVED IN FUTURE STREAMLINING OF PROGRAM
C      NBA     = BACKGROUND SUBTRACT (1=YES,0=NO)
C      NZ      = INITIAL CHANNEL FOR COMPUTATION
C      MF      = FINAL CHANNEL FOR COMPUTATION
C      TB      = COUNTING TIME FOR BACKGROUND
C      Q       = REJECTION COEFFICIENT
C
C      *****
C      D      WRITE      (MO, 901)NS,M,NIT,NBA,NZ,MF
0043      IF(NS)897,897,3
C      *****
C
C
0044      3 JJ=1
0045      DO 10 I=1,NS
0046      IDAT=65+(I-1)*16
```

```
C
C
C      CONTROL PARAMETERS FOR EACH LIBRARY ELEMENT
C
0047      READ(MI' IDAT)TISOT(JJ)
0048      JJ=JJ+1
0049      READ(MI' IDAT)TISOT(JJ)
0050      JJ=JJ+1
0051      IDAT=IDAT+8
0052      READ(MI' IDAT)HA(I)
0053      READ(MI' IDAT)TST(I)
0054      READ(MI' IDAT)AC(I)
C
C      TISOT(JJ) = ISOTOPE NAME (8 CHARACTERS MAX)
C      HA(I)     = HALF-LIFE (SECS.)
C      TST(I)    = COUNTINUE TIME OF STANDARD
C      AC(I)     = ACTIVITY
C
0055      10 CONTINUE
```

```
0056      IF (NBA) 50,50,40
0057      40 IDAT=42
0058      DO 45 J=1,32,4
      C
      C      ASC(I)      =  STANDARD BACKGROUND SPECTRUM (FILE.ELEMENT(,DEVICE))
      C
      C
0059      45 READ(MI,IDAT)ASC(J),ASC(J+1),ASC(J+2),ASC(J+3)
0060      WRITE(MO,902)(ASC(I),I=1,32)
0061      902 FORMAT(1X'STANDARD BACKGROUND: ',32A1)
0062      CALL      GET(ASC,BA,IVAR,FILE,M)
0063      WRITE      (MO,903)(BA(I),I=1,M)
      C
0064      50 DO 130 I=1,NS
0065      IDAT=65+(I-1)*16+2
0066      DO 52 J=1,32,4
      C
      C      ASC(I)      =  STANDARD SPECTRUM (FILE.ELEMENT(,DEVICE))
      C
      C
0067      52 READ(MI,IDAT)ASC(J),ASC(J+1),ASC(J+2),ASC(J+3)
0068      CALL      GET(ASC,S,IVAR,FILE,M)
      C
      C      *XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
0069      IF(NBA) 70,70,60
      C
      C
      C      SUBTRACT BACKGROUND (MULTIPLIED BY COUNT TIME OF STANDARD/ COUNT
      C      TIME OF BACKGROUND) FROM STANDARD
      C
0070      60 FAT=TST(I)/TB
0071      DO 65 J=1,M
0072      S(J)=S(J)-BA(J)*FAT
0073      65 CONTINUE
      C
```

```
C
C      DON'T LET STANDARD COUNTS BE LESS THAN .01
C
0074      70 DO 75 J=1,M
0075          IF(S(J).LT.0.0)S(J)=.01
0077      75 CONTINUE
0078          IF(NBA) 100,100,80
0079      80 WRITE(M0,904)(ASC(II),II=1,32)
0080      904 FORMAT('0','BACKGROUND SUBTRACTED STANDARD: ',32A1)
0081          WRITE(M0,903)(S(J),J=1,M)
0082      100 CONTINUE

C
C      SAVE STANDARD SPECTRUM IN VIRTUAL MEMORY OUT ON DISK
C
0083      IVAR=(I-1)*M+1
0084      DO 120 K=1,M
0085      120 WRITE(10'IVAR)S(K)
0086      130 CONTINUE
0087      170 WRITE              (M0,908)
C      *****
```

```
C
C      CONTROL PARAMETERS FOR UNKNOWN SAMPLE
C
0088      IDAT=12
0089      READ(MIU' IDAT)NBR
0090      READ(MIU' IDAT)NBS
0091      READ(MIU' IDAT)TB
0092      READ(MIU' IDAT)TSA
0093      READ(MIU' IDAT)VRED
0094      READ(MIU' IDAT)DAY
0095      READ(MIU' IDAT)VM

C      (USER DEFINED)
C      NBR      = BACKGROUND SUPPLIED ? (YES=1,NO=0)
C      NBS      = BACKGROUND SUBTRACT ? (YES=1,NO=0)
C      TB       = COUNTING TIME FOR BACKGROUND (SECS)
C      TSA      = COUNTING TIME FOR UNKNOWN SAMPLE (SECS)
C      VRED     = VOLUME REDUCTION FACTOR (INVERSE OF DILUTION FACTOR)
C      DAY      = DECAY TIME (SECS)
C      VM       = RESULT MULTIPLICATION FACTOR
C
C      *XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX*
```

```
0096 180 IF (VM) 190,190,200
0097 190 VM=1.0
0098 200 IF (VRED) 210,210,220
0099 210 VRED=1.0
0100 220 IF (TB) 230,230,240
0101 230 FS=0.0
0102      GO TO 250
0103 240 FS=TSA/TB
0104 250 FX=FS+FS**2
0105      IF(NBR) 270,270,260
0106 260 CONTINUE
      C *****
      C
      C
      C      ASC(JJ) = SAMPLE & BACKGROUND SPECTRUM (FILE.ELEMENT(,DEVICE))
      C
0107      DO 265 JJ=1,32,4
0108 265 READ(MIU' IDAT)ASC(JJ),ASC(JJ+1),ASC(JJ+2),ASC(JJ+3)
      C
      C      WRITE(MD,910)(ASC(I),I=1,32)
0910  FORMAT(1H1,'SAMPLE BACKGROUND: ',32A1)
      C
0109      CALL      GET(ASC,BA,IVAR,FILE,M)
      C      WRITE      (MD,903)(BA(I),I=1,M)
0110 270 CONTINUE
0111      IDAT=2
      C
0112      DO 280 JJ=1,32,4
0113 280 READ(MIU' IDAT)ASC(JJ),ASC(JJ+1),ASC(JJ+2),ASC(JJ+3)
```

```
      C
0114      WRITE(MD,911)(ASC(I),I=1,32)
0115      911 FORMAT(' ','SAMPLE SPECTRUM: ',32A1)
      C
      C
0116      DO 290 I=1,32
0117      290 TNAME(I)=ASC(I)
0118      CALL      GET(ASC,Y,IVAR,FILE,M)
      C
      C      ****
0119      IF (NBS) 310,310,300
0120      300 DO 305 I=1,M
0121      305 Y(I)=Y(I)-BA(I)*FS
0122      310 SB=0.0
0123      DO 320 I=NZ,MF
0124      320 SB=SB+BA(I)
0125      WRITE      (MD,903)(Y(I), I=1,M)
0126      S1=0.0
0127      S2=0.0
0128      DO 330 I=NZ,MF
0129      330 S1=S1+Y(I)
0130      S2=S1+SB*FX
0131      WRITE      (MD, 912)SB,S1
      C
      C
      C      SAVE ORIGINAL SAMPLE SPECTRUM OUT ON DISK
      C
0132      IVAR=(NS+2)*M+1
0133      DO 340 I=1,M
0134      340 WRITE(10,IVAR)Y(I)
      C
```

```
C
C
0135      IDAT=IDAT+18
C
C      UNKNOWN SAMPLE OPTION VARIABLES
C
0136      NB=0
0137      READ(MIU,IDAT)NW
0138      READ(MIU,IDAT)N
0139      READ(MIU,IDAT)F0
0140      READ(MIU,IDAT)LW
0141      READ(MIU,IDAT)NEWST
0142      READ(MIU,IDAT)BR
0143      READ(MIU,IDAT)BP
0144      READ(MIU,IDAT)KRO
0145      DO 350 I=1,32,4
0146 350    READ(MIU,IDAT) ASC(I),ASC(I+1),ASC(I+2),ASC(I+3)
0147      NDET=0

C      (USER DEFINED)
C      NW      = WEIGHTING FACTOR DETERMINATION (BASED ON ACTUAL
C              COUNTS/CHANNEL=0, BASED ON CALCULATED COUNTS/CHN=1)
C      N      = NUMBER OF LIBRARY SPECTRA TO BE FITTED TO SAMPLE
C      F0     = F-TEST REJECTION COEFFICIENT
C      LW     = WEIGHTING FACTOR CALCULATION ((COUNTS)**-1=-1,
C              (SIGMA)**-2=0, 1=1)
C      NEWST  = APPLY REJECTION COEFFICIENT ? (YES=1,NO=0)
C      BR     = BACKGROUND REGRESSION? (TRIAL SET, CHOSEN SET
C              OF STANDARDS=0, BACKGROUND ONLY=0)
C
C      BP     = PIVOT ON BACKGROUND ALLOWED ?
C              =0 NO PIVOT ON BACKGROUND ALLOWED
C              =1 ALLOW PIVOT ON BACKGROUND
C      KRO = OUTPUT RESIDUALS ? (YES=1,NO=0)
C      ASC = FILENAME FOR RESIDUALS
C      IS(I) = NUMBER OF LIBRARY STANDARD TO BE FIT IN ORDER OF
C              DESIRED PRINTOUT
```

```
      C
0148      DO 360 I=1,NS
0149      360 ISL(I)=0
0150      DO 370 I=1,N
0151      READ(MIU,IDAT) IS(I)
0152      370 ISL(I)=IS(I)
      C
0153      DO 380 J=1,N
0154      DO 375 I=1,NS
0155      IF(IS(J)-I) 372,372,375
0156      372 II=2*I-1
      C
      C
      C      STORE IN ARRAY TISO ONLY THOSE LIBRARY NAMES ACTUALLY USED IN THE
      C      LEAST SQUARES FIT
      C
0157      JJ=2*J-1
0158      TISO(JJ)=TISOT(II)
0159      II=II+1
0160      JJ=JJ+1
0161      TISO(JJ)=TISOT(II)
      C
      C      *XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX*
0162      GO TO 380
0163      375 CONTINUE
0164      380 CONTINUE
0165      TISO((N+1)*2-1)=SNAM(1)
0166      TISO((N+1)*2)=SNAM(2)
0167      IS(N+1)=N+1
0168      LN=N+1
```

```
0169      DO 390 J=1,N
0170      390 IT(J)=J
0171      DO 395 I=1,N
0172      IF (IS(I).EQ.1) GO TO 400
0174      395 CONTINUE
0175      WRITE(MO,913)
0176      913 FORMAT('0',5X,45('*')/5X,'*',45X,'*/5X,'*',4X,
X'BACKGROUND NOT INCLUDED AS A STANDARD',4X,'*/
XSX,'*',45X,'*/5X,45('*')/)
0177      400 CONTINUE
0178      IF (BP.EQ.0) GO TO 401
0180      WRITE(MO,936)
0181      401 DO 402 I=1,N
0182      402 EF(I)=.FALSE.

C
C      SET UP ARRAY A(N+1,N+1)
C
0183      405 DO 420 I=1,M
0184      IF (LW) 422,412,410
0185      410 W(I)=1.0
0186      GO TO 420
0187      412 T=Y(I)+8A(I)*FX
0188      IF (T- 1.0) 414,414,416
0189      414 W(I)=1.0
0190      GO TO 420
0191      416 W(I)=1.0/T
0192      420 CONTINUE
0193      GO TO 424
0194      422 DO 423 I=1,M
0195      423 W(I)=1.0/(Y(I)+1.0)
```

C

```
0196      424 SUMW=0.0
0197      DO 425 I=1,M
0198      425 SUMW=SUMW+1.0/W(I)
0199      WRITE(MO,914)
0200      914 FORMAT('0','*'*10'* CORRELATION MATRIX '*10*'/)
0201      ENCODE(17,915,IFORN) LN
0202      915 FORMAT('(14X','I2','(2A4,2X)/)')
0203      WRITE(MO,IFORN) (TISO(I*2-1),TISO(I*2),I=1,LN)
0204      DO 446 L=1,N
0205      N5=IS(L)
0206      IVAR=(N5-1)*M+NZ
0207      DO 435 J=NZ,MF
0208      435 READ(10*IVAR)R(J)
      C
      C      COMPUTE WEIGHTED SUMS OF STANDARD SPECTRA
      C
0209      SS(L)=0.
0210      DO 436 J=NZ,MF
0211      436 SS(L)=SS(L)+R(J)*W(J)
0212      DO 444 K=L,N
0213      N6=IS(K)
0214      IVAR=(N6-1)*M+NZ
0215      DO 437 J=NZ,MF
0216      437 READ(10*IVAR)S(J)
0217      442 SA=0.
```

```
C
C      GET LEAST SQUARES SUM COEFFICIENTS FOR UNKNOWN CONCENTRATIONS Z(I)
C      AND SAMPLE Y(I)
C
0218      DO 443 I=NZ,MF
0219      443 SA=SA+S(I)*R(I)*W(I)
0220      A(K,L)=SA
0221      A(L,K)=A(K,L)
0222      444 CONTINUE
0223      SA=0.
0224      DO 445 I=NZ,MF
0225      SA=SA+R(I)*Y(I)*W(I)
0226      445 CONTINUE
0227      B(L)=SA
0228      A(N+1,L)=SA
0229      A(L,N+1)=A(N+1,L)
0230      446 CONTINUE
0231      SA=0.
0232      DO 450 I=NZ,MF
0233      SA=SA+Y(I)*Y(I)*W(I)
0234      450 CONTINUE
0235      A(LN,LN)=SA
0236      ST=SA
C
C      COMPUTE WEIGHTED SUM OF UNKNOWN
C
0237      SS(LN)=0.
0238      DO 460 J=MZ,NF
0239      460 SS(LN)=SS(LN)+Y(J)*W(J)
```

```
C
C   CALCULATE CORRELATION MATRIX
C
0240      DO 468 L=1, LN
0241      N5=IS(L)
0242      DO 465 K=L, LN
0243      N6=IS(K)
0244      SRD1=A(K,K)-SS(N6)**2/SUMW
0245      SRD2=A(L,L)-SS(N5)**2/SUMW
0246      CC(K,L)=(A(K,L)-SS(N6)*SS(N5)/SUMW)/SQRT(SRD1*SRD2)
0247  465 CONTINUE
0248      LSK=(L-1)*10+2
0249      KAC=LN-L+1
0250      ENCODE(25,916,IFORKL) LSK,KAC
0251  916 FORMAT(' (2X,2A4,',I2,'X,',I2,' (F8.4,2X)/')')
0252      WRITE(MO,IFORKL) TISO(L*2-1),TISO(L*2),(CC(K,L),K=L,LN)
0253  468 CONTINUE
C
C   PRINT OUT WEIGHTED SUMS OF STANDARDS AND UNKNOWN
C
0254      WRITE(MO,905)
0255      WRITE(MO,906) (SS(I),I=1,LN)
```

```
C
C
C
C      DO PIVOTAL REGRESSION ANALYSIS
C
C
C      REGRESSION WITH ALL REQUESTED STANDARDS
C
0256      E=0
0257      P=N
0258      IF(BR.EQ.0) GO TO 479
0260      WRITE(MO,930)
0261      DO 470 I=1,N
0262      IF(ISL(I).EQ.1) GO TO 471
0264      470 CONTINUE
0265      471 N5=ISL(I)
0266      E=E+MY(N5)
0267      CALL PIVOT(A,I,EF,LN)
0268      IPO=1
0269      P=1
0270      GO TO 700
0271      479 DO 480 I=1,P
0272      E=E+MY(IS(I))
0273      CALL PIVOT(A,I,EF,LN)
0274      480 CONTINUE
0275      IPO=1
0276      GO TO 700
C
```

```
C
C      SELECT TRIAL SUBSET OF MATRIX A
C
0277      500 F=E
0278          D=0
0279          IF(BR.EQ.0) GO TO 502
0281          F=0
0282          DO 501 I=1,N
0283              NS=ISL(I)
0284              F=F+MY(NS)
0285      501 CONTINUE
0286          GO TO 609
0287      502 P=N
0288      508 DO 510 I=1,N
0289          NS=ISL(I)
0290          IF(BP.EQ.1) GO TO 509
0292          IF(NS.EQ.1) GO TO 510
0294          IF(STD(I).LE.0.0) GO TO 511
0296      509 IF(Z(I)/STD(I).GE.1.0) GO TO 510
0298      511 CALL PIVOT(A,I,EF,LN)
0299          E=E-MY(NS)
0300          P=P-1
0301      510 CONTINUE
0302          IF(E.EQ.1.AND.Z(1).LT.0.0) GO TO 890
0304          IF(E.GT.0) GO TO 540

C
C      FIND LARGEST F-VALUE AND USE THAT STANDARD AS THE TRIAL SET
C
0306          FPS=0.0
0307          DO 530 I=1,N
0308              IF(Z(I)) 530,530,520
0309      520 IF(FP(I).LT.FPS) GO TO 530
0311              FPS=FP(I)
0312              J=I
0313      530 CONTINUE
0314              P=1
0315              E=E.AND.MY(ISL(J))
0316      540 IPO=2
0317              GO TO 700
```

```
C
C   BACKWARD PIVOT
C
0318 550 C=E
0319 IF(E.EQ.1.AND.BP.EQ.0) GO TO 800
0321 551 FMIN=10000.
0322 DO 555 I=1,N
0323 FPM(I)=1000.
0324 N5=ISL(I)
0325 IF(BP.EQ.1) GO TO 552
0327 IF(N5.EQ.1) GO TO 555
0329 552 IN=C.AND.MY(N5)
0330 IF(IN) 555,555,554
0331 554 FPM(I)=(NCH-P)*((A(I,LN)**2)/(-A(I,I)*A(LN,LN)))
0332 IF(A(I,LN).GT.0.0) FPM(I)=-FPM(I)
0334 IF(FPM(I).GE.FMIN) GO TO 555
0336 FMIN=FPM(I)
0337 J=I
0338 555 CONTINUE
0339 DF=NCH-P
0340 ZS=-A(J,LN)
0341 IF(FMIN.LT.0.0) FMIN=-FMIN
0343 CALL XQCALC(DF,FMIN,ZS,XF,QF,0)
0344 IF(XF.GE.F0) GO TO 560
0346 CALL PIVOT(A,J,EF,LN)
0347 E=E-MY(ISL(J))
0348 P=P-1
0349 560 IPO=3
0350 GO TO 700
0351 600 JDF=F-D
0352 IF(E.EQ.JDF) GO TO 800
```

```
C
C   FORWARD PIVOT
C
0354   609 IF(BR.EQ.1) C=E
0356       D=F-C
0357       IF(D.EQ.0) GO TO 630
0359       FMAX=0.0
0360       DF=NCH-P-1
0361       WRITE(MO,932)
0362       DO 620 I=1,N
0363       FPM(I)=0.0
0364       NS=ISL(I)
0365       IF(BP.EQ.1) GO TO 610
0367       IF(NS.EQ.1) GO TO 620
0369   610 IN=D.AND.MY(NS)
0370       IF(IN) 620,620,615
0371   615 INEG=0
0372       SQUC=A(I,I)*A(LN,LN)
0373       IF(SQUC.GT.0.0) GO TO 616
0375       SQUC=-1.0*SQUC
0376       INEG=1
0377   616 RHO=A(I,LN)/SQRT(SQUC)
0378       IF(INEG.EQ.1) RHO=-1.0*RHO
0380       R2=RHO**2
0381       IF(INEG.EQ.1) R2=-1.0*R2
0383       FPM(I)=DF*R2/(1.0-R2)
0384       ZS=A(I,LN)
0385       FPS=FPM(I)
0386       CALL XDCALC(DF,FPS,ZS,XF,QF,0)
0387       RMSR=A(LN,LN)*(1.0-R2)/DF
0388       WRITE(MO,933) TISO(I*2-1),TISO(I*2),FPS,QF,XF,RHO,RMSR
0389       IF(XF.LT.0.0) FPM(I)=-FPM(I)
0391       IF(FPM(I).LE.FMAX) GO TO 620
0393       FMAX=FPM(I)
0394       J=I
0395   620 CONTINUE
0396       ZS=A(J,LN)
0397       CALL XDCALC(DF,FMAX,ZS,XF,QF,0)
0398       IF(XF.LT.F0) GO TO 630
0400       CALL PIVOT(A,J,EF,LN)
0401       E=E+MY(ISL(J))
0402       P=P+1
0403       IPO=4
0404       BR=0
0405       GO TO 700
0406   630 IF(E.EQ.C) GO TO 800
0408       GO TO 550
```

C  
C  
C

OUTPUT SECTION FOR PARTIAL F,Q,X AND ANALYSIS OF VARIANCE

```
0409 700 J=0
0410 DF=NCH-P
0411 RSS=A(LN, LN)
0412 RMSR=RSS/DF
0413 DO 730 I=1, N
0414 N5=ISL(I)
0415 IN=E.AND.MY(N5)
0416 IF(IN) 730, 730, 720
0417 720 J=J+1
0418 TISOT(2*J-1)=TISOT(2*I-1)
0419 TISOT(2*J)=TISOT(2*I)
0420 Z(J)=-A(I, LN)*TST(N5)/TSA
0421 SQUC=A(I, I)
0422 IF(SQUC.LT.0.0) SQUC=-1.0*SQUC
0424 STD(J)=SQRT(SQUC*RMSR)*TST(N5)/TSA
0425 FP(J)=(Z(J)/STD(J))*2
0426 730 CONTINUE
0427 WRITE(MO, 918) HF(IPO), SNAM(1), SNAM(2)
0428 918 FORMAT('1', 'RESULTS OF ', A8, ' REGRESSION ON ', 2A4, '///')
0429 WRITE(MO, 919) DF, RSS, RMSR
0430 919 FORMAT(' ', 'DEGREES OF FREEDOM=', F11.0/
X13X, 'RSS=', 1PE11.3/13X, 'MSR=', 1PE11.3//)
0431 DO 740 I=1, P
0432 FPS=FP(I)
0433 ZS=Z(I)
0434 CALL XQCALC(DF, FPS, ZS, XF, QF, 0)
0435 FP(I)=XF
0436 RMSR=A(LN, LN)*(1.0+FPS/DF)/(DF+1)
0437 730 WRITE(MO, 920) TISOT(I*2-1), TISOT(I*2), Z(I), STD(I), FPS, QF, XF, RMSR
0438 920 FORMAT(' ', 2X, 2A4, 1PE13.4, 2X, '+', 1PE11.2, 3X, 'F=',
X1PE12.4, 3X, 'Q=', 1PE12.4, 3X, 'X=', 1PE12.4, 3X, 'RMSR=', 1PE12.4)
0439 740 CONTINUE
0440 GO TO (500, 550, 600, 630), IPO
```

```
C
C   FINAL RESULT SECTION
C
0441   800 SG=0
0442       J=0
0443       IF(E.EQ.1.AND.Z(1).LT.0.0) GO TO 890
0445       DO 820 I=1,N
0446           N5=ISL(I)
0447           IN=E.AND.MY(N5)
0448           IF(IN) 820,820,815
0449   815 J=J+1
0450       SG=SG-A(I,LN)*B(I)
0451       TISOT(J*2-1)=TISO(I*2-1)
0452       TISOT(J*2)=TISO(I*2)
0453   820 CONTINUE
```

```
C
C
```

```
C
0454      CH=0.0
0455      VY=0.
0456      VU=0.0
0457      VVV=0.0
0458      JJJ=0

C
C
C      THIS LOOP READS FROM A SCRATCH FILE INTO CORE UP TO 15
C      STANDARDS. 64 CHANNELS AT A TIME SO THAT RESIDUALS AND STANDARD
C      ERRORS MAY BE DETERMINED
C
0459      DO 835 J=NZ,MF
0460      JJJ=JJJ+1
0461      SV=0.
0462      JJ=0
0463      DO 828 I=1,N
0464      N5=ISL(I)
0465      IN=E.AND.MY(N5)
0466      IF(IN) 828,828,822
0467      822 JJ=JJ+1
0468      IF(JJJ.GT.1.AND.JJJ.LT.65)GO TO 827
0470      JJJ=1
0471      LOOP=(MF+1)-J
0472      IF(LOOP.GT.64)LOOP=64
0474      IVAR=(N5-1)*M+J
0475      DO 826 II=1,LOOP
0476      826 READ(10,IVAR)ARR(JJ,II)
D      WRITE(MD,903)(ARR(JJ,II),II=1,LOOP)
0477      827 SV=SV+ARR(JJ,JJJ)*(-A(I,LN))
0478      IF(JJ.EQ.P) JJ=0
0480      828 CONTINUE

C
```

```
      C
0481      RE=Y(J)-SV
0482      T=RE**2
0483      VY=VY+W(J)*T
0484      VU=VU+T
0485      TMO=ABS(0.1+SV)
0486      TMP=TMO+BA(J)*FX
0487      VVV=VVV+TMP
0488      IF (NW) 833,833,830
0489      830 IF (LW) 832,831,833
0490      831 W(J)=1.0/TMP
0491      GO TO 833
0492      832 W(J)=1.0/TMO
0493      833 RT=T/TMP
0494      CH=CH+RT
0495      TMP=SQRT(TMP)

      C
      C
      C      CALCULATES RESIDUALS OVER STANDARD DEVIATION, R(J)
      C
0496      R(J)=RE/TMP
0497      TE=Y(J)+BA(J)*FX
0498      835 CONTINUE
0499      SR=VY
```

```
C
C      CALCULATES NUMBER OF DEGREES OF FREEDOM, DN
C
0500      DN=MF-P-NZ+1
0501      DR=DN
0502      DG=P
0503      DT=DR+DG
0504      CHDF=CH/DN
0505      VY=VY/DN
0506      WRITE(MO,896)
0507      WRITE(MO,934) SNAM(1),SNAM(2)
0508      WRITE              (MO, 921)CHDF
0509      J=0
0510      840 DO 844 I=1,N
0511          NS=ISL(I)
0512          IN=E.AND.MY(NS)
0513          IF(IN) 844,844,841
0514      841 J=J+1
C
C      DECAY CORRECTION DONE HERE
C
0515      FD= EXP(0.693*DAY/HA(NS))
```

```
C
C   CORRECTED STANDARD ERROR DETERMINED FROM THE VARIANCE
C
0516   STD(J)=SQRT(-A(I,I)*A(LN,LN)/DN)*TST(N5)/TSA
0517   STD(J)=AC( N5 )*FD*STD(J)*VM/VRED
C
C   RELATIVE CONCENTRATION IS CONVERTED TO ACTUAL CONCENTRATION LEVEL
C
0518   Z(J)=(-A(I,LN))*(TST(N5)/TSA)*AC(N5)*FD*VM/VRED
0519   844 CONTINUE
C
0520   846   WRITE          (MO,922)
0521   DO 847 I=1,P
0522   FPS=(Z(I)/STD(I))*2
0523   ZPS=Z(I)
0524   CALL XQCALC(DN,FPS,ZPS,XF,QF,0)
0525   RMSR=A(LN,LN)*(1.0+FPS/DR)/(DR+1)
0526   WRITE(MO,920) TISOT(I*2-1),TISOT(I*2),Z(I),STD(I),FPS,QF,XF,RMSR
0527   847 CONTINUE
C
C   WRITE ANALYSIS OF VARIANCE TABLE
C
0528   XG=SG/DG
0529   XR=SR/DR
0530   FF=XG/XR
0531   WRITE(MO,924)HH
0532   WRITE(MO,925)HG,DG,SG,XG,FF
0533   WRITE(MO,925)HR,DR,SR,XR
0534   WRITE(MO,925)HT,DT,ST
C
C   COMPUTE LLNL R-STATISTIC
C
0535   CALL RSTAT(NCH,P,R,NZ,MF)
```

```
C
C      COMPUTE FINAL STATISTICS FOR STANDARDS ELIMINATED
C      DURING PIVOTAL REGRESSION
C
0536      WRITE(MO,935)
0537      DF=NCH-P-1
0538      J=0
0539      DO 850 I=1,N
0540      N5=ISL(I)
0541      IN=D.AND.MY(N5)
0542      IF(IN) 850,850,848
0543      848 J=J+1
0544      TISOT(J*2-1)=TISO(I*2-1)
0545      TISOT(J*2)=TISO(I*2)
0546      ZS=A(I,LN)
0547      INEG=0
0548      SQUC=A(I,I)*A(LN,LN)
0549      IF(SQUC.GT.0.0) GO TO 849
0551      SQUC=-1.0*SQUC
0552      INEG=1
0553      849 RHO=A(I,LN)/SQRT(SQUC)
0554      IF(INEG.EQ.1) RHO=-1.0*RHO
0556      R2=RHO**2
0557      IF(INEG.EQ.1) R2=-1.0*R2
0559      FPS=DF*R2/(1.0-R2)
0560      CALL XQCALC(DN,FPS,ZS,XF,QF,0)
0561      RMSR=A(LN,LN)*(1.0-R2)/DF
0562      WRITE(MO,933) TISOT(J*2-1),TISOT(J*2),FPS,QF,XF,RHO,RMSR
0563      850 CONTINUE
0564      WRITE              (MO,926) SNAM(1),SNAM(2)
0565      DO 851 II=1,NZ-1
0566      851 R(II)=0.0
0567      WRITE              (MO,927) (R(J),J=1,MF)
0568      853 K=0
0569      N2=MF-2
C
```

```
C
C      FIND SUSPICIOUS CHANNELS. THESE ARE DEFINED AS CHANNELS WHERE
C      STD/RESIDUAL IS GREATER THAN 10 OR WHERE STD/RESIDUAL IS GREATER
C      THAN 2 FOR THE CHANNELS ON EITHER SIDE OF THE ONE CONSIDERED.
C
0570      DO 870 J=NZ,N2
0571          T=ABS(R(J))
0572          IF(T-10.) 860,860,866
0573      860 IF(R(J-1)-2.0 ) 870,862,862
0574      862 IF(R(J)-2.0 ) 870,864,864
0575      864 IF(R(J+1)-2.0 ) 870,866,866
0576      866 K=K+1
0577          IR(K)=J
0578          SIR(K)=R(J)
0579          IF(K.GT.50) GO TO 872
0581      870 CONTINUE
0582      872 WRITE              (MO,928)
0583          WRITE              (MO,929)(IR(I),SIR(I),I=1,K)
0584          CALL RESID(R,NZ,MF)
0585          CALL RUNS(R,NZ,MF)
0586          IF(KRO.NE.1) GO TO 880
0588          DO 876 I=NZ,MF
0599              R(I)=R(I)*100+1000
0590              IF(R(I).GT.2000.) R(I)=2000.
0592              IF(R(I).LT.0.) R(I)=0.
0594      876 CONTINUE
0595          CALL PUT(ASC,R,IVAR,FILE,M)
0596      880 GO TO 895
```

C

```
0597 901 FORMAT(' ',1X,6I4)
0598 903 FORMAT (2X,7F8.0)
0599 905 FORMAT('0',1X,'WEIGHTED SUMS OF STANDARDS AND UNKNOWN',/)
0600 906 FORMAT(1X,1PE11.4,1PE11.4,1PE11.4,1PE11.4,/)
0601 908 FORMAT(1H0)
0602 909 FORMAT(3A2,2X, 12,15,13,12,110, 5E10.3)
0603 912 FORMAT(1H1,'BACKGD SUM=',1PE12.3,' SAMPLE SUM=',1PE12.3,/)
0604 921 FORMAT(' ',1X,'FIT=',1PE11.3)
0605 922 FORMAT(1H0,'RESULTS=CONCENTRATIONS AND EST STANDARD ERRORS',/)
0606 926 FORMAT(1H1,' RATIO OF RESIDUALS OVER STD DEV PER CHANNEL FOR',
X1X,2A4,/)
0607 927 FORMAT (1X,F7.1, 6F8.1)
0608 928 FORMAT(1H0,'SUSPICIOUS CHANNELS',/)
0609 929 FORMAT (5(I4,2X,F5.2),/)
0610 924 FORMAT(1H0,12X,'ANALYSIS OF VARIANCE'/1X,2A4,6X,A4,4X,3(A4,7X))
0611 925 FORMAT(1X,A8,F11.0,1P4E11.3)
0612 930 FORMAT(' ',14X,40('*')/15X,'*',8X,
1'STARTING ANALYSIS WITH',8X,'*/15X,'*',5X,
2'TRIAL SET = BACKGROUND ONLY',6X,'*/15X,
340('*'))
0613 932 FORMAT(' ',//////////
1' CALCULATED PARTIAL F-,Q- AND X-VALUES TO ADD:')
0614 933 FORMAT(' ',2A4,3X,'F=',1PE12.4,3X,'Q=',1PE12.4,
13X,'X=',1PE12.4,3X,'RHO=',1PE12.4,3X,'AMSR=',1PE12.4)
0615 934 FORMAT(' ',50('*')/13X,'FINAL RESULT FOR ',2A4,/50('*')//)
0616 935 FORMAT(' ',////////' FINAL STATISTICS FOR ELIMINATED STANDARDS')
0617 936 FORMAT(' ',10X,41('*')/11X,'*',5X,
1'PIVOT ON BACKGROUND PERMITTED',5X,'*/11X,41('*'))
0618 890 WRITE(MD,940)
0619 WRITE(7,940)
0620 940 FORMAT(' NONE OF THE CHOSEN STANDARDS RESULT'/
X'IN A SIGNIFICANT CONTRIBUTION TO THE'/
X'BACKGROUND SUBTRACTED SAMPLE SPECTRUM')
0621 895 WRITE(MD,896)
0622 896 FORMAT('1')
0623 897 CONTINUE
0624 END
```

## MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
A	000006	REAL*4 ARRAY (10,10) VECTORED
Y	000626	REAL*4 ARRAY (513)
Z	004632	REAL*4 ARRAY (10)
S	004702	REAL*4 ARRAY (512)
STD	011702	REAL*4 ARRAY (10)
B	011752	REAL*4 ARRAY (10)
R	012022	REAL*4 ARRAY (512)
W	016022	REAL*4 ARRAY (512)
IR	022022	INTEGER*2 ARRAY (512)
MY	026022	INTEGER*2 ARRAY (10)
FPM	026046	REAL*4 ARRAY (10)
FP	026116	REAL*4 ARRAY (10)
BA	022022	REAL*4 ARRAY (512)
SS	026166	REAL*4 ARRAY (10)
AC	026236	REAL*4 ARRAY (10)
HA	026306	REAL*4 ARRAY (10)
IS	026356	INTEGER*2 ARRAY (10)
TST	026402	REAL*4 ARRAY (10)
HAT	026452	REAL*4 ARRAY (10)
TNAME	026522	LOGICAL*1 ARRAY (36)
TISOT	026566	REAL*4 ARRAY (40)
TISO	027026	REAL*4 ARRAY (20)
IT	027146	INTEGER*2 ARRAY (10)
SNAM	026530	REAL*4 ARRAY (2)
ARR	004702	REAL*4 ARRAY (10,64) VECTORED
HH	027172	REAL*4 ARRAY (6)
SIR	027222	REAL*4 ARRAY (50)
ISL	027532	INTEGER*2 ARRAY (10)
HF	027556	REAL*8 ARRAY (4)
IFORM	027616	INTEGER*2 ARRAY (20)
IFORKL	027666	INTEGER*2 ARRAY (30)
CC	027762	REAL*4 ARRAY (10,10) VECTORED
ASC	030602	LOGICAL*1 ARRAY (60)
DEF	030676	LOGICAL*1 ARRAY (10)
EF	030710	LOGICAL*1 ARRAY (10)
HG	030722	REAL*8 VARIABLE
HR	030732	REAL*8 VARIABLE
HT	030742	REAL*8 VARIABLE
C	034016	INTEGER*2 VARIABLE
D	034020	INTEGER*2 VARIABLE
E	030752	INTEGER*2 VARIABLE
F	034022	INTEGER*2 VARIABLE
P	034024	INTEGER*2 VARIABLE
BR	034026	INTEGER*2 VARIABLE
BP	034030	INTEGER*2 VARIABLE
FILE	034032	INTEGER*2 VARIABLE
TIS1	030754	REAL*4 VARIABLE
TIS2	030760	REAL*4 VARIABLE
IDAT	034034	INTEGER*2 VARIABLE
IVAR	034036	INTEGER*2 VARIABLE
MI	034040	INTEGER*2 VARIABLE
MIU	034042	INTEGER*2 VARIABLE
MO	034044	INTEGER*2 VARIABLE
I	034046	INTEGER*2 VARIABLE
NNN	034050	INTEGER*2 VARIABLE
IPO	034052	INTEGER*2 VARIABLE
NS	034054	INTEGER*2 VARIABLE

## MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
M	034056	INTEGER*2 VARIABLE
NIT	034060	INTEGER*2 VARIABLE
NBA	034062	INTEGER*2 VARIABLE
NZ	034064	INTEGER*2 VARIABLE
MF	034066	INTEGER*2 VARIABLE
TB	034070	REAL*4 VARIABLE
Q	034074	REAL*4 VARIABLE
NCH	034100	INTEGER*2 VARIABLE
JJ	034102	INTEGER*2 VARIABLE
J	034104	INTEGER*2 VARIABLE
GET	000000	REAL*4 PROCEDURE
FAT	034106	REAL*4 VARIABLE
II	034112	INTEGER*2 VARIABLE
K	034114	INTEGER*2 VARIABLE
NBR	034116	INTEGER*2 VARIABLE
NBS	034120	INTEGER*2 VARIABLE
TSA	034122	REAL*4 VARIABLE
VRED	034126	REAL*4 VARIABLE
DAY	034132	REAL*4 VARIABLE
VM	034136	REAL*4 VARIABLE
FS	034142	REAL*4 VARIABLE
FX	034146	REAL*4 VARIABLE
SB	034152	REAL*4 VARIABLE
S1	034156	REAL*4 VARIABLE
S2	034162	REAL*4 VARIABLE
NB	034166	INTEGER*2 VARIABLE
NW	034170	INTEGER*2 VARIABLE
N	034172	INTEGER*2 VARIABLE
F0	034174	REAL*4 VARIABLE
LW	034200	INTEGER*2 VARIABLE
NEWST	034202	INTEGER*2 VARIABLE
KRO	034204	INTEGER*2 VARIABLE
NDET	034206	INTEGER*2 VARIABLE
LN	034210	INTEGER*2 VARIABLE
T	034212	REAL*4 VARIABLE
SUMW	034216	REAL*4 VARIABLE
L	034222	INTEGER*2 VARIABLE
N5	034224	INTEGER*2 VARIABLE
N6	034226	INTEGER*2 VARIABLE
SA	034230	REAL*4 VARIABLE
ST	034234	REAL*4 VARIABLE
MZ	034240	INTEGER*2 VARIABLE
NF	034242	INTEGER*2 VARIABLE
SRD1	034244	REAL*4 VARIABLE
SRD2	034250	REAL*4 VARIABLE
SQRT	000000	REAL*4 PROCEDURE
LSK	034254	INTEGER*2 VARIABLE
KAC	034256	INTEGER*2 VARIABLE
PIVOT	000000	REAL*4 PROCEDURE
FPS	034260	REAL*4 VARIABLE
FMIN	034264	REAL*4 VARIABLE
IN	034270	INTEGER*2 VARIABLE
DF	034272	REAL*4 VARIABLE
ZS	034276	REAL*4 VARIABLE
XDCALC	000000	REAL*4 PROCEDURE
XF	034302	REAL*4 VARIABLE
QF	034306	REAL*4 VARIABLE

# MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
JDF	034312	INTEGER*2 VARIABLE
FMAX	034314	REAL*4 VARIABLE
INEG	034320	INTEGER*2 VARIABLE
SQUC	034322	REAL*4 VARIABLE
RHO	034326	REAL*4 VARIABLE
R2	034332	REAL*4 VARIABLE
RMSR	034336	REAL*4 VARIABLE
RSS	034342	REAL*4 VARIABLE
SG	034346	REAL*4 VARIABLE
CH	034352	REAL*4 VARIABLE
VY	034356	REAL*4 VARIABLE
VU	034362	REAL*4 VARIABLE
VVV	034366	REAL*4 VARIABLE
JJJ	034372	INTEGER*2 VARIABLE
V	034374	REAL*4 VARIABLE
LOOP	034400	INTEGER*2 VARIABLE
RE	034402	REAL*4 VARIABLE
TMO	034406	REAL*4 VARIABLE
ABS	000000	REAL*4 PROCEDURE
TMP	034412	REAL*4 VARIABLE
RT	034416	REAL*4 VARIABLE
TE	034422	REAL*4 VARIABLE
SR	034426	REAL*4 VARIABLE
DN	034432	REAL*4 VARIABLE
DR	034436	REAL*4 VARIABLE
DG	034442	REAL*4 VARIABLE
DT	034446	REAL*4 VARIABLE
CHDF	034452	REAL*4 VARIABLE
FD	034456	REAL*4 VARIABLE
EXP	000000	REAL*4 PROCEDURE
ZPS	034462	REAL*4 VARIABLE
XG	034466	REAL*4 VARIABLE
XR	034472	REAL*4 VARIABLE
FF	034476	REAL*4 VARIABLE
RSTAT	000000	REAL*4 PROCEDURE
N2	034502	INTEGER*2 VARIABLE
RESID	000000	REAL*4 PROCEDURE
RUNS	000000	REAL*4 PROCEDURE
PUT	000000	REAL*4 PROCEDURE
<hr/>		
COMMON BLOCK /X		LENGTH 000004
FUD	000000	REAL*4 VARIABLE

ND 6600 LINKER V02-A-1 LOAD MAP 5 OCT 1983 1:43:12 PM

SECTION	ADDR	SIZE	ENTRY	ADDR	ENTRY	ADDR	ENTRY	ADDR
. ABS.	000000	000000	\$LRECL	000210	\$NLCHN	000006	\$USRSW	000000
			\$RF183	000000				
. ABS.	000000	000000	\$SYSLB	000000				
. ABS.	000000	000000	\$TRACE	004737				
. ABS.	000000	000000	\$V004A	000001				
\$. \$\$. \$.	020000	000000	\$. \$\$. \$.	020000				
X &	020000	000004	X	020000				
	020004	053706						
	073712	001066	PIVOT	073712				
	075000	001060	RSTAT	075000				
	076060	000624	XQCALC	076060				
	076704	000552	GET	076704				
	077456	000614	PUT	077456				
	100272	001364	RESID	100272				
	101656	001342	RUNS	101656				
	103220	000772	HISTO	103220				
	104212	000106	CONCAT	104212				
	104320	000060	NMI\$II	104320	NMI\$MI	104346	NMI\$PI	104354
			NPI\$II	104364	NPI\$MI	104370	NPI\$PI	104374
	104400	000044	NMI\$1P	104400	NPI\$1I	104420	NPI\$1M	104432
			NPI\$1P	104414				
	104444	000142	SQRT	104444				
	104606	000350	EXP	104606				
	105156	000262	XFI\$	105156	\$PWRI	105156		
	105440	000110	TAD\$	105470	TAF\$	105476	TAI\$	105440
			TAL\$	105446	TAP\$	105462	TAQ\$	105454
	105550	000056	\$OTIS	105550				
	105626	000210	ISN\$	105626	LSN\$	105646	\$ISNTR	105632
			\$LSNTR	105652				
	106036	000034	END\$	106036	ERR\$	106054		
	106072	000046	EOL\$	106072				
	106140	000044	RET\$	106154	RET\$F	106144	RET\$I	106152
			RET\$L	106140				
	106204	001106	IBR\$	106212	IBW\$	106204	\$IBW	106216
	107312	000072	ENC\$	107312				
	107404	000020	IFR\$	107404	IFW\$	107416		
	107424	001562	\$FIO	110112				
	111206	002344	DCO\$	112632	ECO\$	112624	FCO\$	112620
			GCO\$	112612	ICI\$	111214	ICO\$	112366
			OCI\$	111206	OCO\$	112360	RCI\$	111410
			\$GET	111374				
	113552	000110	\$DUMPL	113552				
	113662	000036	\$GETFI	113662				
	113720	000042	DII\$IS	113732	DII\$MS	113726	DII\$PS	113720
			DII\$SS	113734	\$DVI	113734		
	113762	000040	MUI\$IS	113774	MUI\$MS	113770	MUI\$PS	113762
			MUI\$SS	113776	\$MLI	113776		
	114022	000130	CIC\$	114022	CID\$	114022	CIF\$	114032
			CIL\$	114144	CLC\$	114022	CLD\$	114022
			CLF\$	114032	CLI\$	114150	\$DI	114022
			\$RI	114032				

114152	000120	\$FCHNL	114152				
114272	000044	BEQ\$	114312	BGE\$	114322	BGT\$	114320
		BLE\$	114310	BLT\$	114332	BNE\$	114330
		BRAS	114324	NMI\$1I	114302	NMI\$1M	114272
114336	000002	\$AOTS	114336				
114340	000100	CCI\$	114340	CDI\$	114340	CFI\$	114354
		\$IC	114340	\$ID	114340	\$IR	114354
114440	000012	\$WAIT	114440				
114452	000026	SAL\$IP	114452	SAL\$MP	114470	SAL\$SP	114454
		SVL\$IP	114460	SVL\$MP	114474	SVL\$SP	114462
114500	000026	SAL\$IM	114500	SAL\$MM	114516	SAL\$SM	114502
		SVL\$IM	114506	SVL\$MM	114522	SVL\$SM	114510
114526	000044	JMC\$	114534	JMI\$M	114530	JMI\$P	114526
114572	000030	AND\$	114576	EQV\$	114604	IOR\$	114572
		XOR\$	114606				
114622	000014	AIF\$	114622				
114636	000036	CAI\$	114636	CAL\$	114644		
114674	000016	ABS	114674				
114712	000102	MOI\$IA	114736	MOI\$IM	114732	MOI\$IS	114726
		MOI\$MA	114752	MOI\$MM	114746	MOI\$MS	114742
		MOI\$SA	114722	MOI\$SM	114716	MOI\$SS	114712
		MOI\$OA	114766	MOI\$OM	114762	MOI\$OS	114756
		MOI\$IA	115006	MOI\$IM	115000	MOI\$IS	114772
		MOL\$IS	114726	MOL\$SS	114712	REL\$	114726
115014	000046	CMI\$IP	115014	CMI\$MP	115024	CMI\$PI	115046
		CMI\$PM	115054	CMI\$PP	115034	CMI\$PS	115040
		CMI\$SP	115016				
115062	000044	CMI\$II	115102	CMI\$IM	115106	CMI\$IS	115076
		CMI\$MI	115116	CMI\$MM	115122	CMI\$MS	115112
		CMI\$SI	115066	CMI\$SM	115072	CMI\$SS	115062
115126	000034	DCI\$A	115156	DCI\$M	115150	DCI\$P	115154
		DCI\$S	115144	ICI\$A	115140	ICI\$M	115132
		ICI\$P	115136	ICI\$S	115126		
115162	000046	SUI\$IP	115162	SUI\$MP	115176	SUI\$PA	115222
		SUI\$PM	115214	SUI\$PP	115172	SUI\$PS	115206
		SUI\$SP	115164				
115230	000044	SUI\$IA	115250	SUI\$IM	115254	SUI\$IS	115244
		SUI\$MA	115264	SUI\$MM	115270	SUI\$MS	115260
		SUI\$SA	115234	SUI\$SM	115240	SUI\$SS	115230
115274	000046	ADI\$IP	115274	ADI\$MP	115310	ADI\$PA	115334
		ADI\$PM	115326	ADI\$PP	115304	ADI\$PS	115320
		ADI\$SP	115276				
115342	000044	ADI\$IA	115362	ADI\$IM	115366	ADI\$IS	115356
		ADI\$MA	115376	ADI\$MM	115402	ADI\$MS	115372
		ADI\$SA	115346	ADI\$SM	115352	ADI\$SS	115342
115406	000064	MOI\$IP	115406	MOI\$MP	115422	MOI\$PA	115446
		MOI\$PM	115440	MOI\$PP	115416	MOI\$PS	115432
		MOI\$SP	115410	MOI\$OP	115454	MOI\$IP	115462
115472	000174	CMF\$II	115546	CMF\$IM	115630	CMF\$IP	115600
		CMF\$IS	115512	CMF\$MI	115536	CMF\$MM	115620
		CMF\$MP	115570	CMF\$MS	115476	CMF\$PI	115532
		CMF\$PM	115614	CMF\$PP	115564	CMF\$PS	115472
		CMF\$SI	115552	CMF\$SM	115634	CMF\$SP	115604
		CMF\$SS	115520	\$CMR	115520		

115666	000116	MOL\$IA	115766	MOL\$IM	115760	MOL\$IP	115774
		MOL\$MA	115712	MOL\$MM	115706	MOL\$MP	115730
		MOL\$MS	115676	MOL\$PA	115752	MOL\$PM	115740
		MOL\$PP	115724	MOL\$PS	115746	MOL\$SA	115672
		MOL\$SM	115666	MOL\$SP	115716		
116004	000026	MOF\$RA	116022	MOF\$RM	116012	MOF\$RP	116026
		MOF\$RS	116004				
116032	000012	MOF\$SS	116032				
116044	000014	MOF\$IS	116044	MOF\$OS	116052		
116060	000016	MOF\$MS	116060	MOF\$PS	116072		
116076	000014	MOF\$SA	116076				
116112	000010	MOF\$IA	116112				
116122	000014	MOF\$SM	116122	MOF\$SP	116132		
116136	000020	MOF\$IM	116136	MOF\$IP	116150		
116156	000020	MOF\$OA	116166	MOF\$OM	116156	MOF\$OP	116172
116176	000042	MOF\$MA	116210	MOF\$MM	116176	MOF\$MP	116216
		MOF\$PA	116230	MOF\$PM	116224	MOF\$PP	116234
116240	000054	SAI\$PM	116240	SAI\$PP	116266	SVI\$PM	116252
		SVI\$PP	116300				
116314	000032	SAI\$IP	116314	SAI\$MP	116336	SAI\$SP	116316
		SVI\$IP	116324	SVI\$MP	116342	SVI\$SP	116326
116346	000032	SAI\$IM	116346	SAI\$MM	116370	SAI\$SM	116350
		SVI\$IM	116356	SVI\$MM	116374	SVI\$SM	116360
116400	000032	TSD\$I	116420	TSD\$M	116414	TSD\$P	116424
		TSD\$S	116404	TSF\$I	116420	TSF\$M	116414
		TSF\$P	116424	TSF\$S	116410	TSI\$I	116420
		TSI\$M	116414	TSI\$P	116424	TSI\$S	116400
116432	000034	CPD\$SM	116454	CPF\$SM	116442	CPI\$SM	116436
		CPL\$SM	116432				
116466	000030	LEQ\$	116470	LGE\$	116500	LGT\$	116476
		LLE\$	116466	LLT\$	116512	LNE\$	116510
116516	000024	TSL\$I	116526	TSL\$M	116522	TSL\$P	116534
		TSL\$S	116516				
116542	000044	SAF\$IP	116542	SAF\$MP	116576	SAF\$SP	116544
		SVF\$IP	116554	SVF\$MP	116602	SVF\$SP	116556
116606	000044	SAF\$IM	116606	SAF\$MM	116642	SAF\$SM	116610
		SVF\$IM	116620	SVF\$MM	116646	SVF\$SM	116622
116652	000036	NGD\$A	116704	NGD\$M	116664	NGD\$P	116700
		NGD\$S	116652	NGF\$A	116704	NGF\$M	116664
		NGF\$P	116700	NGF\$S	116652		
116710	000044	SAD\$IM	116710	SAD\$MM	116744	SAD\$SM	116712
		SYD\$IM	116724	SYD\$MM	116750	SYD\$SM	116726
116754	000030	MOD\$MS	116764	MOD\$PS	116760	MOD\$SS	116754
		MOD\$VS	116766				
LUND	117004	000054	LUNDEF	117004			
CLOSU	117060	000032	CLOSEU	117060			
\$M. TVT	117112	000062	TVD\$	117126	TVF\$	117120	TVI\$
			TVL\$	117112	TVP\$	117142	TVQ\$
OT	117174	001510	\$ERR\$S	117704	\$FPERR	117546	\$OTI
STOP	120704	000112	EXIT	120730	FOO\$	120704	STP\$
RIO	121016	000600	DEF\$	121532	IRR\$	121016	IRW\$
			\$GETIN	121402			
GETREC	121616	000346	\$GETRE	121616	\$TTYIN	122116	
ENDFIL	122164	000042	EOF\$	122164			

CLOSE	122226	000550	\$CLOSE	122226			
OUTREC	122776	000414	\$PUTRE	122776			
\$M.FIO	123412	000216	\$FMTDR	123412	\$FMTDW	123446	\$INITI 123520
OPEN	123630	000610	\$OPEN	123630			
FADD	124440	000062	ADF\$IS	124440	ADF\$MS	124452	ADF\$PS 124446
			ADF\$SS	124444	SUF\$IS	124466	SUF\$MS 124500
			SUF\$PS	124474	SUF\$SS	124472	\$ADR 124444
			\$SBR	124472			
FDIV	124522	000034	DIF\$IS	124540	DIF\$MS	124526	DIF\$PS 124522
			DIF\$SS	124544	\$DVR	124544	
FMUL	124556	000034	MUF\$IS	124574	MUF\$MS	124562	MUF\$PS 124556
			MUF\$SS	124600	\$MLR	124600	
RWBLK	124612	000460	\$EOFIL	125222	\$GETBL	125034	\$PUTBL 124612
ERRTB	125272	000100	\$ERRTB	125272			
ERRS	125372	002570	\$ERRS	125372			
\$M.LCV	130162	000106	LCI\$	130162	LCO\$	130230	
ADDM	130270	000116	ADF\$IM	130270	ADF\$IM	130302	ADF\$PM 130276
			ADF\$SM	130312	SUF\$IM	130326	SUF\$PM 130362
			SUF\$PM	130356	SUF\$SM	130334	
ADDP	130406	000114	ADF\$IP	130406	ADF\$IP	130420	ADF\$PP 130414
			ADF\$SP	130430	SUF\$IP	130444	SUF\$PP 130500
			SUF\$PP	130474	SUF\$SP	130452	
ADDA	130522	000150	ADF\$IA	130522	ADF\$IA	130554	ADF\$PA 130550
			ADF\$SA	130532	SUF\$IA	130600	SUF\$PA 130634
			SUF\$PA	130630	SUF\$SA	130606	\$FPA 130574
			\$FPA	130654			
\$M.LNO	130672	000022	COL\$S	130672	COL\$A	130702	COL\$M 130676
			COL\$P	130706	COL\$S	130672	

# SEGMENT PARAMETER TABLE

SEG SIZE LIMIT  
0 110714 130714

PROGRAM SIZE = 110714  
DATA AREA SIZE = 000000  
TRANSFER ADDRESS = 020004  
STACK SIZE = 001000

```
0001      SUBROUTINE HISTO(LABEL,IH,XL,XD,N)
          C      WRITTEN BY G.PHILLIPS JUNE 1981
          C
0002      REAL*8 LABEL(4)
0003      LOGICAL*1 A(50),ASTAR,ACOLON
0004      DIMENSION IH(21)
0005      DATA A/50*1H*/,IOUT/6/
0006      DATA ASTAR/1H*/,ACOLON/1H:/
          C
0007      MAX=0
0008      DO 200 K=1,N
0009      200  IF(MAX.LE.IH(K)) MAX=IH(K)
0011      IDIV=1
0012      L=5
0013      250  IF(MAX/IDIV.LE.50) GO TO 300
0015      IDIV=IDIV*2
0016      IF(IDIV.LT.L) GO TO 250
0018      IDIV=L*2
0019      L=L*10
0020      GO TO 250
0021      300  IDELT=IDIV/2
0022      WRITE(IOUT,310) LABEL
0023      310  FORMAT(1H1,4A8)
0024      WRITE(IOUT,320) IDIV
0025      320  FORMAT(1H0,'SCALE FACTOR=',I6/)
0026      X=XL
0027      IT=0
0028      DO 400 K=1,N
0029      IT=IT+IH(K)
0030      J=(IH(K)+IDELT)/IDIV
0031      IF(J.LT.1) A(1)=ACOLON
0033      WRITE(IOUT,360) X,IH(K),(A(I),I=1,J)
0034      360  FORMAT(1X,G11.3,I8,2X,50A1)
0035      A(1)=ASTAR
0036      X=X+XD
0037      400  CONTINUE
0038      WRITE(IOUT,410) IT
0039      410  FORMAT(1H0,4X,'TOTAL =',I8)
0040      DO 500 I=1,5
0041      500  WRITE(IOUT,510)
0042      510  FORMAT(1H0)
0043      RETURN
0044      END
10038      IF(RE1.LT.0.)RE1=32768.+RE1
0040      IF(RE1.GE.16384.)RE1=RE1-16384.
0042      ARRAY(K)=RE1*65536.+RE2
0043      100  CONTINUE
0044      K=M+1
0045      END FILE FILE
0046      200  M=K-1
0047      RETURN
0048      END
```

# MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
------	--------	------------

LABEL	000014	REAL*8 PARAMETER ARRAY (4)
A	000026	LOGICAL*1 ARRAY (50)
IH	000016	INTEGER*2 PARAMETER ARRAY (21)
XL	000020	REAL*4 PARAMETER VARIABLE
XD	000022	REAL*4 PARAMETER VARIABLE
N	000024	INTEGER*2 PARAMETER VARIABLE
ASTAR	000112	LOGICAL*1 VARIABLE
ACOLON	000113	LOGICAL*1 VARIABLE
IOUT	000110	INTEGER*2 VARIABLE
MAX	000210	INTEGER*2 VARIABLE
K	000212	INTEGER*2 VARIABLE
IDIV	000214	INTEGER*2 VARIABLE
L	000216	INTEGER*2 VARIABLE
IDELT	000220	INTEGER*2 VARIABLE
X	000222	REAL*4 VARIABLE
IT	000226	INTEGER*2 VARIABLE
J	000230	INTEGER*2 VARIABLE
I	000232	INTEGER*2 VARIABLE
000234	REAL*4	VARIABLE
RE3	000238	REAL*4 VARIABLE

COMMON BLOCK /HEAD/ LENGTH 000142

IHDR	000000	INTEGER*2 VARIABLE
TITLE	000002	INTEGER*2 ARRAY (32)
ID	000102	INTEGER*2 ARRAY (8)
ELTIME	000122	REAL*4 VARIABLE
PLTIME	000126	REAL*4

```
0001      SUBROUTINE PIVOT(A,P,E,K)
      C
      C      WRITTEN BY: G. W. PHILLIPS AND B. G. GLAGOLA JULY, 1982  NRL
      C
      C      REFERENCE: M. J. GARSIDE, APPL. STAT. 20(1971) 111-112
      C
0002      INTEGER P1,P2,P
0003      REAL A(10,10)
0004      LOGICAL*1 E(10)
      C      DIMENSION N MUST BE GREATER THAN OR EQUAL K.
      C      ARRAY E MUST BE INITIALIZED ".FALSE." BEFORE
      C      FIRST CALL TO PIVOT.
      C
0005      AA=1.0/A(P,P)
0006      A(P,P)=-AA
0007      P1=P-1
0008      P2=P+1
0009      IF(P.EQ.1) GO TO 350
0010      DO 300 I=1,P1
0011          AIP=A(I,P)*AA
0012          DO 100 J=I,P1
0013              A(I,J)=A(I,J)-AIP*A(J,P)
0014      100 CONTINUE
0015          DO 200 J=P2,K
0016              A(I,J)=A(I,J)-AIP*A(P,J)
0017      200 CONTINUE
0018          A(I,P)=-AIP
0019          IF(E(P)) A(I,P)=AIP
0020      300 CONTINUE
0021      350 DO 500 I=P2,K
0022          AIP=A(P,I)*AA
0023          DO 400 J=I,K
0024              A(I,J)=A(I,J)-AIP*A(P,J)
0025      400 CONTINUE
0026          A(P,I)=-AIP
0027          IF(E(P)) A(P,I)=AIP
0028      500 CONTINUE
0029      E(P)=.NOT.E(P)
0030      RETURN
0031      END
0032      IF(RE1.LT.0.)RE1=32768.+RE1
0033      IF(RE1.GE.16384.)RE1=RE1-16384.
0034      ARRAY(K)=RE1*65536.+RE2
0035      100 CONTINUE
0036      K=M+1
0037      END FILE FILE
0038      200 M=K-1
0039      RET.
0040      END
```

# MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
A	000014	REAL*4 PARAMETER ARRAY (10,10) VECTORED
E	000020	LOGICAL*1 PARAMETER ARRAY (10)
P	000016	INTEGER*2 PARAMETER VARIABLE
K	000022	INTEGER*2 PARAMETER VARIABLE
P1	000050	INTEGER*2 VARIABLE
P2	000052	INTEGER*2 VARIABLE
AA	000054	REAL*4 VARIABLE
I	000060	INTEGER*2 VARIABLE
AIP	000062	REAL*4 VARIABLE
J	000066	INTEGER*2 VARIABLE

```
0001      SUBROUTINE GET(ASC,ARRAY,IVAR,FILE,M)
          C      LAST MODIFIED OCTOBER 1982 BY G.W.P.
          C
0002      COMMON/HEAD/IHDR,TITLE(32),ID(8),ELTIME,PLTIME,ERTIME,PRTIME
0003      INTEGER*2 TITLE,ID
0004      DIMENSION ARRAY(256),ITIME(4)
0005      LOGICAL*1 ASC(60),DEF(10),NAM(60)
0006      INTEGER FILE
0007      DEFINE FILE FILE(0,2,U,IVAR)
0008      ENCODE(8,10,DEF)FILE
0009      10  FORMAT('DEF ',12,' ')
0010      DEF(9)=.FALSE.
0011      DEF(10)=.FALSE.
0012      CALL CONCAT(DEF,ASC,NAM,59)
0013      CALL LUNDEF(NAM,E)
0014      IVAR=12
0015      DO 12 I=1,4
0016      12  READ(FILE*IVAR)MLT,ITIME(I)
0017      PLTIME=ITIME(1)
0018      ELTIME=ITIME(2)
0019      PRTIME=ITIME(3)
0020      ERTIME=ITIME(4)
0021      IVAR=84
0022      DO 20 I=1,31,2
0023      20  READ(FILE*IVAR)TITLE(I),TITLE(I+1)
0024      DO 30 I=1,7,2
0025      30  READ(FILE*IVAR)ID(I),ID(I+1)
0026      IHDR=1
0027      IVAR=28
0028      READ(FILE*IVAR)A0
0029      READ(FILE*IVAR)B0
0030      READ(FILE*IVAR)C0
0031      IVAR=193
0032      DO 100 K=1,M
0033      READ(FILE*IVAR,END=200)MSB,LSB
0034      RE1=MSB
0035      RE2=LSB
0036      IF(RE2.LT.0.)RE2=65536.+RE2
0038      IF(RE1.LT.0.)RE1=32768.+RE1
0040      IF(RE1.GE.16384.)RE1=RE1-16384.
0042      ARRAY(K)=RE1*65536.+RE2
0043      100  CONTINUE
0044      K=M+1
0045      END FILE FILE
0046      200  M=K-1
0047      RETURN
0048      END
```

# MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
ARRAY	000016	REAL*4 PARAMETER ARRAY (256)
ITIME	000026	INTEGER*2 ARRAY (4)
ASC	000014	LOGICAL*1 PARAMETER ARRAY (60)
DEF	000036	LOGICAL*1 ARRAY (10)
NAM	000050	LOGICAL*1 ARRAY (60)
IVAR	000020	INTEGER*2 PARAMETER VARIABLE
FILE	000022	INTEGER*2 PARAMETER VARIABLE
M	000024	INTEGER*2 PARAMETER VARIABLE
CONCAT	000000	REAL*4 PROCEDURE
LUNDEF	000000	INTEGER*2 PROCEDURE
E	000172	REAL*4 VARIABLE
I	000176	INTEGER*2 VARIABLE
MLT	000200	INTEGER*2 VARIABLE
A0	000202	REAL*4 VARIABLE
B0	000206	REAL*4 VARIABLE
C0	000212	REAL*4 VARIABLE
K	000216	INTEGER*2 VARIABLE
MSB	000220	INTEGER*2 VARIABLE
LSB	000222	INTEGER*2 VARIABLE
RE1	000224	REAL*4 VARIABLE
RE2	000230	REAL*4 VARIABLE

COMMON BLOCK /HEAD/ LENGTH 000142

IHDR	000000	INTEGER*2 VARIABLE
TITLE	000002	INTEGER*2 ARRAY (32)
ID	000102	INTEGER*2 ARRAY (8)
ELTIME	000122	REAL*4 VARIABLE
PLTIME	000126	REAL*4 VARIABLE
ERTIME	000132	REAL*4 VARIABLE
PRTIME	000136	REAL*4 VARIABLE

```
0001      SUBROUTINE PUT(ASC,ARRAY,IVAR,FILE,M)
          C      WRITTEN BY G. PHILLIPS, JUNE 1981
          C
0002      DIMENSION ARRAY(256)
0003      LOGICAL*1 ASC(60),DEF(10),NAM(60)
0004      INTEGER FILE
0005      DEFINE FILE FILE(448,2,U,IVAR)
0006      ENCODE(8,10,DEF)FILE
0007      10  FORMAT('DEF ',I2,', ')
0008      DEF(9)=.FALSE.
0009      DEF(10)=.FALSE.
0010      CALL CONCAT(DEF,ASC,NAM,59)
0011      CALL LUNDEF(NAM,E)
0012      IVAR=193
0013      DO 100 K=1,M
0014      V=ARRAY(K)
0015      IF(V.LT.0.) V=0.
0017      IF(V.LT.65536.) GOTO 50
0019      V=V/65536.
0020      IF(V.GT.16383.) V=16383.
0022      MSB=V
0023      LSB=0
0024      GOTO 80
0025      50  IF(V.GT.32767.) V=V-65536.
0027      LSB=V
0028      MSB=0
0029      80  WRITE(FILE*IVAR)MSB,LSB
0030      100 CONTINUE
0031      END FILE FILE
0032      CALL CLOSEU(FILE)
0033      RETURN
0034      END
A0038      IF(RE1.LT.0.)RE1=32768.+RE1
0040      IF(RE1.GE.16384.)RE1=RE1-16384.
0042      ARRAY(K)=RE1*65536.+RE2
0043      100 CONTINUE
0044      K=M+1
0045      END FILE FILE
0046      200 M=K-1
0047      RETURN
0048      END
```

# MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
ARRAY	000016	REAL*4 PARAMETER ARRAY (256)
ASC	000014	LOGICAL*1 PARAMETER ARRAY (60)
DEF	000026	LOGICAL*1 ARRAY (10)
NAM	000040	LOGICAL*1 ARRAY (60)
IVAR	000020	INTEGER*2 PARAMETER VARIABLE
FILE	000022	INTEGER*2 PARAMETER VARIABLE
M	000024	INTEGER*2 PARAMETER VARIABLE
CONCAT	000000	REAL*4 PROCEDURE
LUNDEF	000000	INTEGER*2 PROCEDURE
E	000172	REAL*4 VARIABLE
K	000176	INTEGER*2 VARIABLE
V	000200	REAL*4 VARIABLE
MSB	000204	INTEGER*2 VARIABLE
LSB	000206	INTEGER*2 VARIABLE
CLOSEU	000000	REAL*4 PROCEDURE
000050		INTEGER*2 VARIABLE
P2	000052	INTEGER*2 VARIABLE
AA	000054	REAL*4 VARIABLE
I	000060	INTEGER*2 VARIABLE
AIP	000062	REAL*4 VARIABLE
J	000066	INTEGER*2 VARIABLE

```
0001 SUBROUTINE RESID(R,NZ,MF)
      C WRITTEN BY G.PHILLIPS JUNE 1981
      C
0002 DIMENSION R(256),A(4),C(4),IH(21)
0003 REAL*8 LABEL(4)
0004 DATA IOUT/6/
0005 DATA LABEL/8H DIST,8HTRIBUTION,8H OF RESI,8HDUALS /
      C
0006 DO 100 K=1,21
0007 100 IH(K)=0
0008 DO 150 J=1,4
0009 150 C(J)=0.
0010 DO 200 I=NZ,MF
0011 DO 180 J=1,4
0012 180 C(J)=C(J)+R(I)*KJ
0013 K=R(I)*2.+11.5
0014 IF(K.GT.21) K=21
0016 IF(K.LT.1) K=1
0018 IH(K)=IH(K)+1
0019 200 CONTINUE
0020 M=MF-NZ+1
0021 DO 220 J=1,4
0022 220 C(J)=C(J)/M
0023 U=C(1)
0024 A(1)=U
0025 U2=U*U
0026 U3=U*U2
0027 U4=U*U3
0028 V=C(2)-U2
0029 A(2)=V
0030 A(3)=C(3)-3*U*C(2)+2*U3
0031 A(4)=C(4)-4*U*C(3)+6*U2*C(2)-3*U4
0032 SD=SQRT(V)
0033 SQ=A(3)/SD**3
0034 EX=A(4)/V**2-3.
      D WRITE(IOUT,1000)M,(1,A(1),C(1),I=1,4)
D1000 FORMAT(1H0,'NUMBER OF ELEMENTS =',I4/
      D 1 (15,2G11.3))
0035 WRITE(IOUT,300)U,V,SQ,EX
0036 300 FORMAT(1H0,'MEAN RESIDUAL =',F8.3,', VARIANCE =',F8.3,
      1 ', SKEWNESS =',G11.3,', EXCESS =',G11.3)
0037 XL=-5.0
0038 XD=0.5
0039 N=21
0040 CALL HISTO(LABEL,IH,XL,XD,N)
0041 RETURN
0042 END
```

# MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES	
R	000014	REAL*4	PARAMETER ARRAY (256)
A	000022	REAL*4	ARRAY (4)
C	000042	REAL*4	ARRAY (4)
IH	000062	INTEGER*2	ARRAY (21)
LABEL	000134	REAL*8	ARRAY (4)
NZ	000016	INTEGER*2	PARAMETER VARIABLE
MF	000020	INTEGER*2	PARAMETER VARIABLE
IOUT	000174	INTEGER*2	VARIABLE
K	000306	INTEGER*2	VARIABLE
J	000310	INTEGER*2	VARIABLE
I	000312	INTEGER*2	VARIABLE
M	000314	INTEGER*2	VARIABLE
U	000316	REAL*4	VARIABLE
U2	000322	REAL*4	VARIABLE
U3	000326	REAL*4	VARIABLE
U4	000332	REAL*4	VARIABLE
V	000336	REAL*4	VARIABLE
SD	000342	REAL*4	VARIABLE
SQRT	000000	REAL*4	PROCEDURE
SQ	000346	REAL*4	VARIABLE
EX	000352	REAL*4	VARIABLE
XL	000356	REAL*4	VARIABLE
XD	000362	REAL*4	VARIABLE
N	000366	INTEGER*2	VARIABLE
HISTO	000000	REAL*4	PROCEDURE

```
0001      SUBROUTINE RSTAT(NCH,P,R,NZ,MF)
      C      WRITTEN BY T. B. GOSNELL 22 JUNE, 1982    LLNL
      C      MODIFIED FOR PREGA BY B. G. GLAGOLA 20 JULY, 1982  NRL
      C
      C      THIS PROGRAM ANALYSES RESIDUALS FROM PREGA, COMPUTES A
      C      A RESIDUAL STATISTIC, ITS EXPECTATION VALUE, STANDARD
      C      DEVIATION AND AN APPROXIMATE ASSOCIATED FAP.
      C
      C      REFERENCE:  A. AARNIO, M. J. KOSKELO AND P. ZOMBORI,
      C                  NUCLEAR INSTR. AND METH. 184(487)1981.
      C
0002      DIMENSION R(512)
0003      REAL NRMR
0004      INTEGER P
0005      CH=NCH
0006      EP=P
0007      DF=CH-EP
0008      MF1=MF-1
0009      RSTT=0
0010      DO 10 I=NZ,MF1
0011         RSTT=RSTT+R(I)*R(I+1)
0012 10  CONTINUE
0013         RSTT=RSTT+R(1)*R(MF)
0014         RSTT=RSTT/DF
0015         EXRES=-EP/CH
0016         SIGRES=SQRT(CH)/DF
0017         NRMR=(RSTT-EXRES)/SIGRES
0018         CALL XQCALC(DF,0.,1.,NRMR,0,1)
0019         WRITE(6,50)
0020 50  FORMAT(' ',////' *XXXXXXXXX LLNL R-STATISTIC *XXXXXXXXX')
0021         WRITE(6,51) RSTT,EXRES,SIGRES,NRMR,Q
0022 51  FORMAT('0', 'AUTO-CORRELATION COEFFICIENT',17(' '),1PE12.4/
      1' EXPECTATION VALUE',28(' '),1PE12.4/
      2' STANDARD DEVIATION',27(' '),1PE12.4/
      3' EQUIVALENT NORMAL STANDARD DEVIATIONS',8(' '),1PE12.4/
      4' R-STAT FAP',35(' '),1PE12.4)
0023      RETURN
0024      END
```

# MIDAS FORTRAN IV STORAGE MAP

NAME	OFFSET	ATTRIBUTES
R	000020	REAL*4 PARAMETER ARRAY (512)
NCH	000014	INTEGER*2 PARAMETER VARIABLE
P	000016	INTEGER*2 PARAMETER VARIABLE
NZ	000022	INTEGER*2 PARAMETER VARIABLE
MF	000024	INTEGER*2 PARAMETER VARIABLE
NRMR	000404	REAL*4 VARIABLE
CH	000410	REAL*4 VARIABLE
EP	000414	REAL*4 VARIABLE
DF	000420	REAL*4 VARIABLE
MF1	000424	INTEGER*2 VARIABLE
RSTT	000426	REAL*4 VARIABLE
I	000432	INTEGER*2 VARIABLE
EXRES	000434	REAL*4 VARIABLE
SIGRES	000440	REAL*4 VARIABLE
SQRT	000000	REAL*4 PROCEDURE
XDCALC	000000	REAL*4 PROCEDURE
Q	000444	REAL*4 VARIABLE
LE		
EX	000352	REAL*4 VARIABLE
XL	000356	REAL*4 VARIABLE
XD	000362	REAL*4 VARIABLE
N	000366	INTEGER*2 VARIABLE
HISTO	000000	REAL*4 PROCEDURE

```
0001      SUBROUTINE RUNS(R,NZ,MF)
          C      WRITEN BY G.PHILLIPS JUNE 1981
          C
0002      DIMENSION R(256),IH(21),NCH(50),KSI(12),NRS(50)
0003      REAL*8 LABEL(4)
0004      DATA LABEL/8H      DI,8HSTRIBUTI,8HON OF RU,8HNS /
0005      DATA KSI/-10,-9,-8,-7,-6,-5,5,6,7,8,9,10/
          C
0006      DO 100 K=1,21
0007      100  IH(K)=0
0008      I=NZ
0009      J=0
          C
0010      200  K=0
0011      ICH=I
0012      210  IF(R(I).LT.0.) GOTO 300
0014      K=K+1
0015      I=I+1
0016      IF(I.GT.MF) GOTO 400
0018      IF(R(I).GE.0.) GOTO 210
0020      GOTO 400
0021      300  K=K-1
0022      I=I+1
0023      IF(I.GT.MF) GOTO 400
0025      IF(R(I).LE.0.) GOTO 300
          C
0027      400  K=K+11
0028      IF(K.LT.1) K=1
0030      IF(K.GT.21) K=21
0032      IH(K)=IH(K)+1
0033      IF(K.GT.6.AND.K.LT.16) GO TO 450
0035      IF(K.GT.6) K=K-9
0037      J=J+1
0038      NCH(J)=ICH
0039      NRS(J)=KSI(K)
0040      450  IF(I.LE.MF) GO TO 200
          C
0042      XL=-10.0
0043      XD=1.0
0044      N=21
0045      CALL HISTO(LABEL,IH,XL,XD,N)
0046      WRITE(6,500)
0047      500  FORMAT(' ',5X,'LOCATIONS AND SIZES OF LARGE RUNS'//)
0048      WRITE(6,501) (NCH(I),NRS(I),I=1,J)
0049      501  FORMAT(' ',5(5X,I4,I6))
0050      RETURN
0051      END
```

# MIDAS FORTRAN IV STORAGE MAP

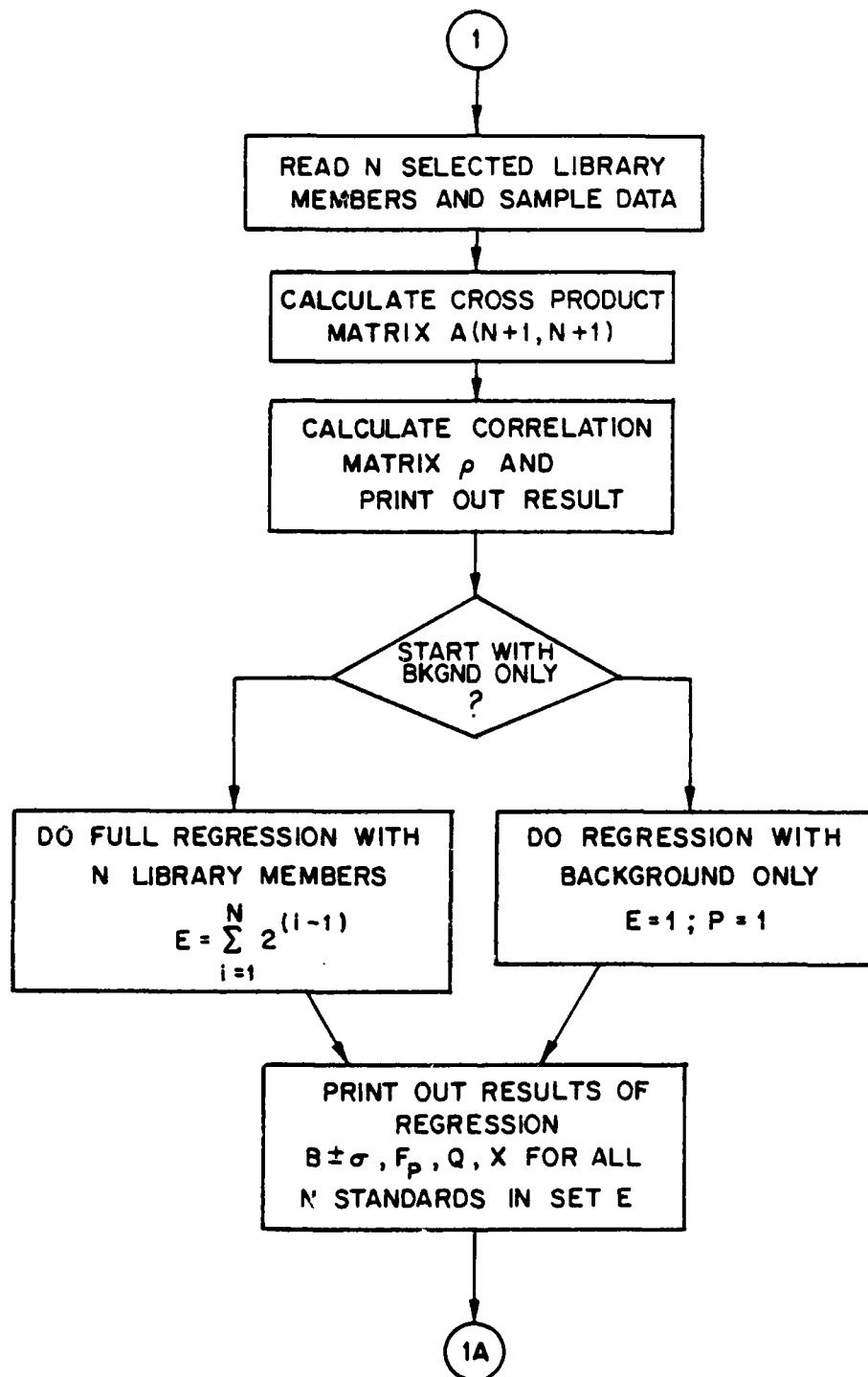
NAME	OFFSET	ATTRIBUTES
R	000014	REAL*4 PARAMETER ARRAY (256)
IH	000022	INTEGER*2 ARRAY (21)
NCH	000074	INTEGER*2 ARRAY (50)
KSI	000240	INTEGER*2 ARRAY (12)
NRS	000270	INTEGER*2 ARRAY (50)
LABEL	000434	REAL*8 ARRAY (4)
NZ	000016	INTEGER*2 PARAMETER VARIABLE
MF	000020	INTEGER*2 PARAMETER VARIABLE
K	000564	INTEGER*2 VARIABLE
I	000566	INTEGER*2 VARIABLE
J	000570	INTEGER*2 VARIABLE
ICH	000572	INTEGER*2 VARIABLE
XL	000574	REAL*4 VARIABLE
XD	000600	REAL*4 VARIABLE
N	000604	INTEGER*2 VARIABLE
HISTO	000000	REAL*4 PROCEDURE
LE		
EX	000352	REAL*4 VARIABLE
XL	000356	REAL*4 VARIABLE
XD	000362	REAL*4 VARIABLE
N	000366	INTEGER*2 VARIABLE
HISTO	000000	REAL*4 PROCEDURE

```
0001      SUBROUTINE XQCALC(DF,F,ZS,X,Q,IEN)
      C
      C      WRITTEN BY B. G. GLAGOLA  JUNE, 1982  NRL
      C
      C      THIS ROUTINE CALCULATES X(F) AND Q(X) GIVEN F
      C
0002      IF(IEN.EQ.1) GO TO 40
0004      DF2=2.*DF-1
0005      IF(F.GT.DF2) GO TO 50
0007      X=(SQRT(F)*(1.-1./(4.*DF)))/(SQRT(1.-F/(2.*DF)))
0008  40  IF(X.GT.12.9) GO TO 60
0010      Z=0.398942*EXP(-X**2/2.)
0011      T=1.0/(1.0+0.33267*X)
0012      Q=Z*(.436184*T-.120168*T**2+.937298*T**3)
0013      GO TO 70
0014  50  X=9.9999E09
0015  60  Q=0.00
0016  70  IF(ZS.LT.0.0) Q=1.-Q
0018      IF(ZS.LT.0.0)X=-X
0020      RETURN
0021      END
0022  400 K=K+11
0028      IF(K.LT.1) K=1
0030      IF(K.GT.21) K=21
0032      IH(K)=IH(K)+1
0033      IF(K.GT.6.AND.K.LT.16) GO TO 450
0035      IF(K.GT.6) K=K-9
0037      J=J+1
0038      NCH(J)=ICH
0039      NRS(J)=KSI(K)
0040  450 IF,J)
0049  501 FORMAT(' ',5(5X,I4,I6))
0050      RETURN
0051      END
```

# MIDAS FORTRAN IV STORAGE MAP

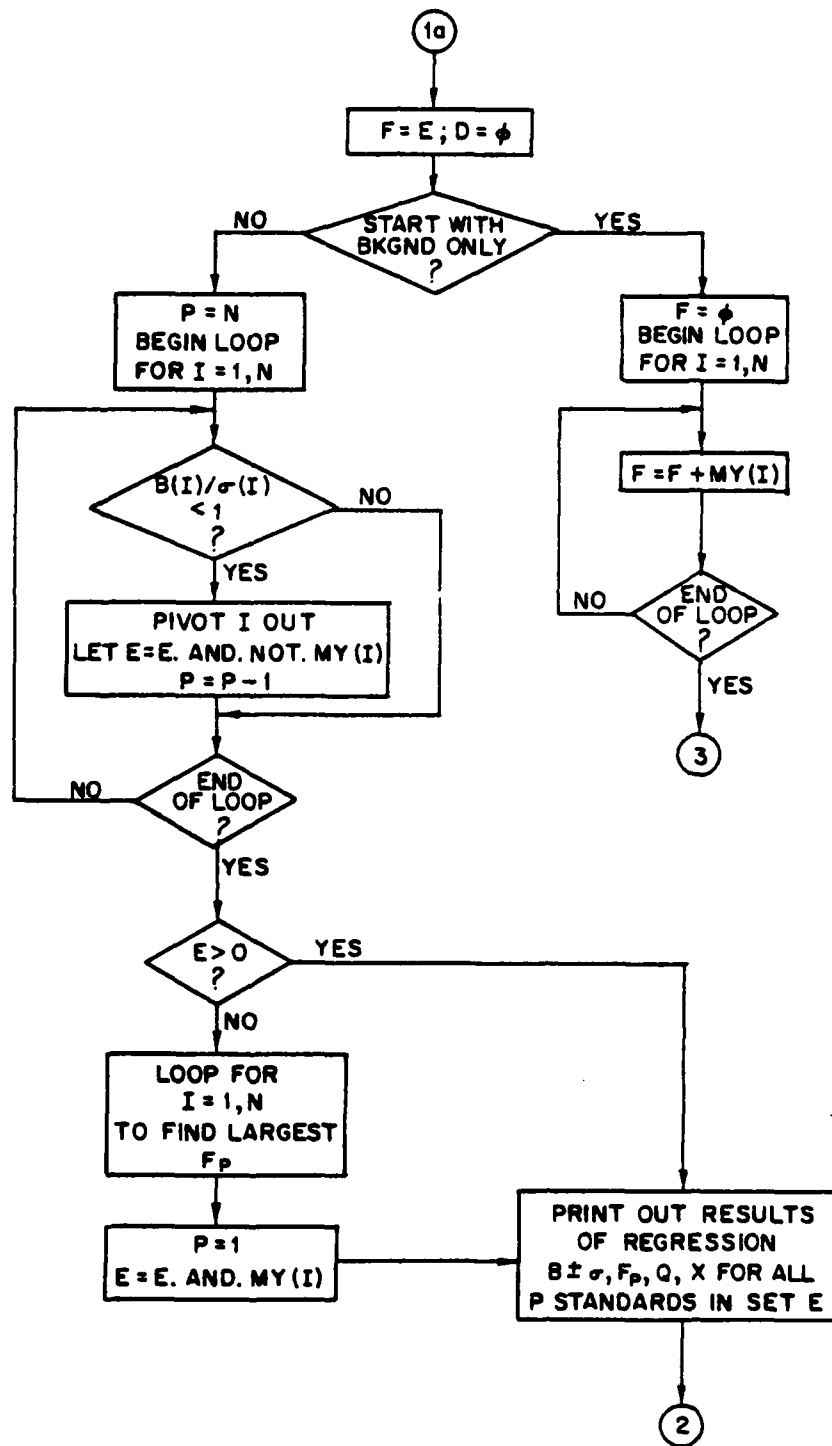
NAME	OFFSET	ATTRIBUTES
DF	000014	REAL*4    PARAMETER VARIABLE
F	000016	REAL*4    PARAMETER VARIABLE
ZS	000020	REAL*4    PARAMETER VARIABLE
X	000022	REAL*4    PARAMETER VARIABLE
Q	000024	REAL*4    PARAMETER VARIABLE
IEN	000026	INTEGER*2 PARAMETER VARIABLE
DF2	000064	REAL*4    VARIABLE
SQRT	000000	REAL*4    PROCEDURE
Z	000070	REAL*4    VARIABLE
EXP	000000	REAL*4    PROCEDURE
T	000074	REAL*4    VARIABLE

# PREGA SETUP

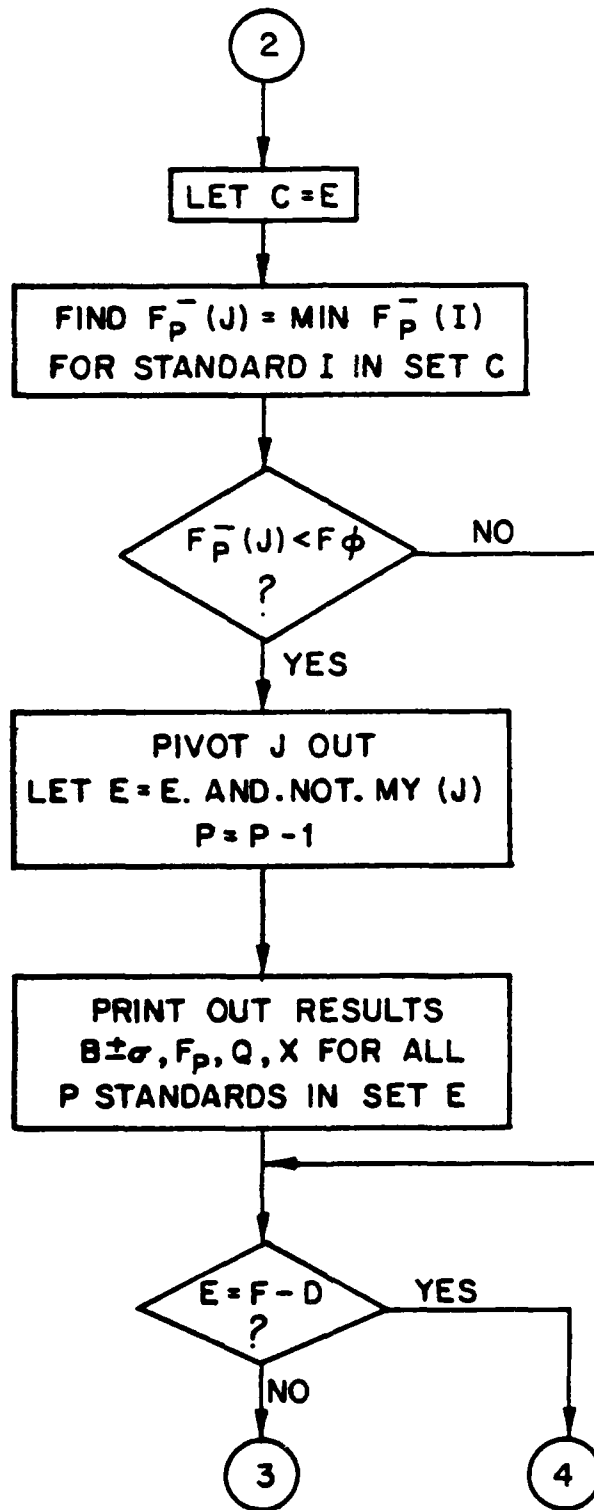


Flow Chart for the Program PREGA showing details of the Major Sections Given in Figure 1.

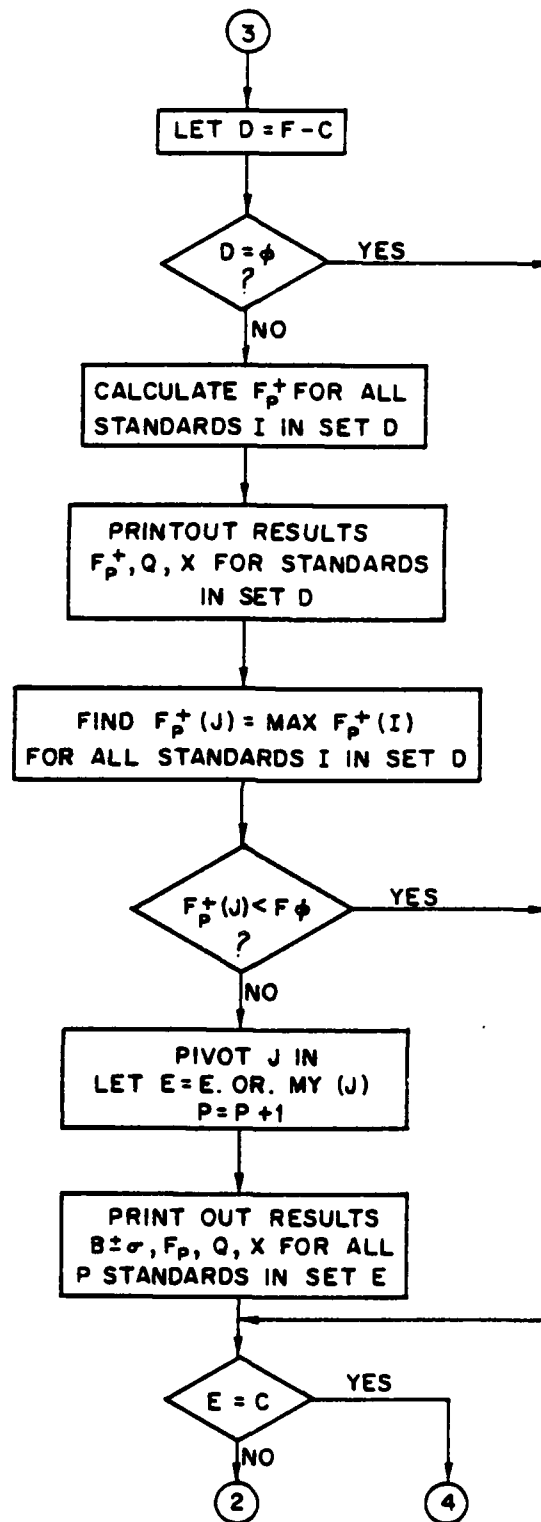
# SELECT TRIAL SUBSET



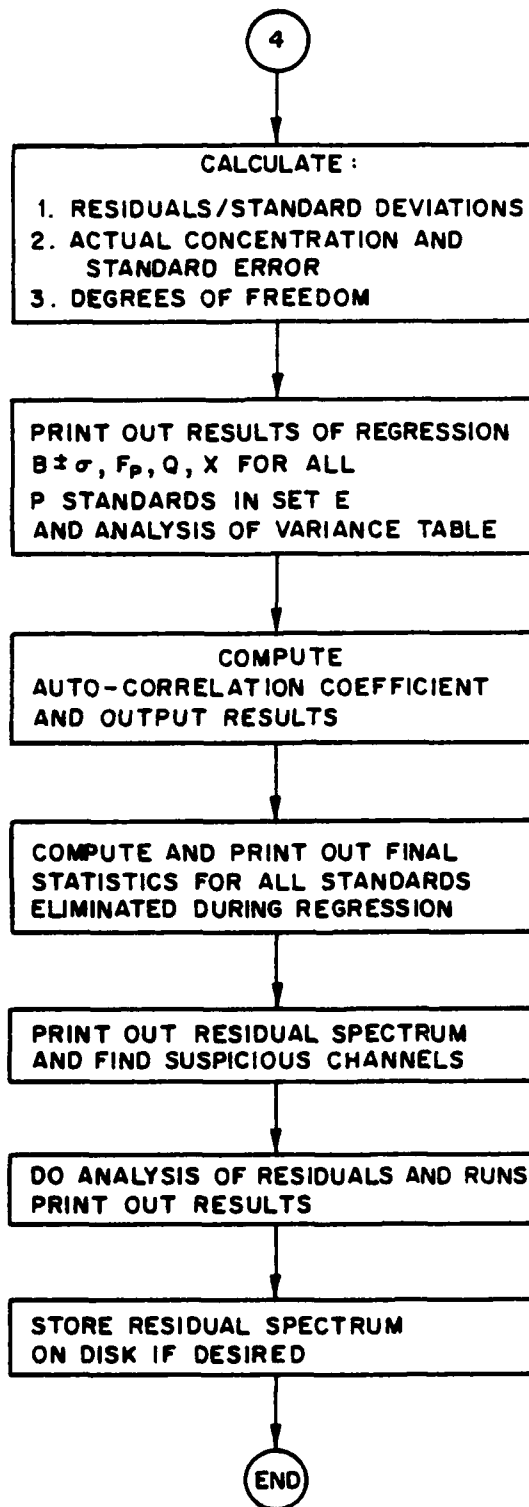
# BACKWARD PIVOT



# FORWARD PIVOT



FINAL RESULTS



## Appendix C: MIDAS System Subroutines

1. ATIME
2. MTAPEF
3. CLOSEU
4. CONCAT
5. LUNDEF

## ATIME (ASCII Date/Time) Subroutine

The ATIME subroutine is used to return the ASCII date and time to the FORTRAN user. This subroutine is written in assembler.

### Form

CALL ATIME (string)

String is the name of the 24 byte string to receive the ASCII date/time. The returned string is 24 bytes in length in the following format:

dd-mmm-yyyy hh:mm:ss xx

where:

dd	Day (number)
mmm	First three letters of the month
yyyy	Year (number)
hh	Hour of the day (12 hours)
mm	Minutes after the hour
ss	Seconds after the minute
xx	AM or PM

NOTE: If the parameter count is <1 or >1, then a return is made to MIDAS.

### Example

LOGICAL\*1 STRING(24)

.  
.  
.

CALL ATIME(STRING)

.  
.  
.

## MTAPEF (FORMATTED MAGNETIC TAPE) SUBROUTINE

The MTAPEF subroutine controls the magnetic tape and its related functions. The subroutine is compatible with either 7 or 9 track magnetic tape. This subroutine is written in Assembler.

### Form

CALL MTAPEF (a,b,c,d,e)

where:

a = Command: INTEGER\*2 variable (required argument).

- = 1 - Initialize control formatter (a,b).
- = 2 - Transport off-line (a,b).
- = 3 - Rewind (a,b).
- = 4 - Search for logical EOT (a,b).
- = 5 - Search for file (a,b,c).
- = 6 - Search for record (a,b,c).
- = 7 - Read one record (a,b,c,d,e).
- = 8 - Verify one record (a,b,c,d,e).
- = 9 - Write one record (a,b,c,d).
- = 10 - Not used.
- = 11 - Over write one record (a,b,c,d).
- = 12 - Dump one record (a,b,c,d).
- = 13 - Write one filemark (a,b).
- = 14 - Write a logical EOT (a,b).
- = 15 - Open transport (a,b,c).
- = 16 - Close transport (a,b).
- = 17 - Tagword (a,b,c,d)

b = Error Number: INTEGER\*2 variable (required).

- = 1 - No error.
- = 2 - Transport assigned to other/or no user.
- = 3 - Magnetic tape transport number error.
- = 4 - Segment is read only.
- = 5 - Segment is not accessible for I/O.
- = 6 - Memory is not contiguous.
- = 7 - Cross segments have different status.
- = 8 - No filemark detected for last operation.
- = 9 - Filemark detected during last operation.
- = 10 - Located on or past physical EOT.
- = 11 - Record read less than list word #14.
- = 12 - Record read greater than list word #14.
- = 13 - Invalid or undefined OP code.
- = 14 - Data late.
- = 15 - Invalid password.
- = 16 - Motion error.
- = 17 - Verification error.
- = 18 - Write protect error.
- = 19 - Parity CRC or LRC error during read.
- = 20 - Operation attempt on off-line transport.
- = 21 - No logical EOT detected during operation.

- = 22 - Logical EOT detected during operation.
- = 23 - Magnetic tape not off-line.
- = 24 - Undefined error bit in status.
- = 25 - Executive error during operation.
- = 26 - Illegal number of arguments.
- = 27 - Illegal command number.
- = 28 - Record length greater than 513 bytes for 7 track transport.

c = Command Parameter 1: INTEGER\*2 variable.

<u>Command Number</u>	<u>Parameter</u>
5	# files to skip
6	# records to skip
7	# bytes to skip
8	# bytes to skip
9	# bytes to write
11	# bytes to write
12	# bytes to write
15	# transport to open
17	Subcommand code (c)
	c = 1 - Get tagword
	c = 2 - Increment tagword
	c = 3 - Put tagword

d = Command Parameter 2: INTEGER\*2 variable or array name.

<u>Command Number</u>	<u>Parameter</u>
7	# bytes to read
8	# bytes to verify
9	Array name to write
11	Array name to write
12	Array name to write
17	Get, Increment, or Put tagword

e = Command parameter 3: Integer variable.

<u>Command Number</u>	<u>Parameter</u>
7	Array name to read
8	Array name to verify

The following is a test program for MTAPEF. The program does the following things:

1. Opens transport.
2. Initializes magnetic tape controller.
3. Reads from the disk and writes to the tape 4096 channels in groups of 128 channels.

4. Writes logical end of tape (of double filemark).
5. Rewinds tape.
6. Reads from tape and writes to disk 4096 channels in groups of 128 channels.
7. Rewinds tape.
8. Closes transport.

```

C      PROGRAM TO TEST MAG TAPE OPERATIONS
C      USING FORTRAN EXTENSION LIBRARY SUBROUTINE
C
C      INTEGER ARRAY (513) A,B,C,D
C      DEFINE FILE 12(4096,2,U,IVAR)
C
C      OPEN FILE
C
C      A=15
C      C=1
C      CALL MTAPEF(A,B,C)
C      IF(B.NE.1)WRITE(6,110)B
C
C      INITIALIZE MAG TAPE
C
C      A=1
C      CALL MTAPEF(A,B)
C      IF(B.NE.1)WRITE(6,100)B
C
C      NOW READ THE DISK & WRITE TO MAG TAPE
C
C      A=9
C      C=513
C      IVAR=129
C      DO 200 I=1,16
C      DO 300 J=1,512,2
300    READ(12,IVAR)ARRAY(J),ARRAY(J+1)
C      CALL MTAPEF(A,B,C,ARRAY)
C      IF(B.NE.1)WRITE(6,120)B
200    CONTINUE
C
C      WRITE A DOUBLE FILEMARK
C
C      A=14
C      CALL MTAPEF(A,B)
C      IF(B.NE.1)WRITE(6,130)B
C
C      REWIND TAPE
C
C      A=3
C      CALL MTAPEF(A,B)
C      IF (B.NE.1)WRITE(6,140)B

```

```

C
C
C      NOW READ FROM TAPE & WRITE TO DISK

      A=7
      C=0
      D=513
      IVAR=129
      DO 400 I=1,16
      CALL MTAPEF(A,B,C,D,ARRAY)
      IF(B.NE.1)WRITE(6,150)B
      DO 500 J=1,512,2
500    READ(12,IVAR)ARRAY(J),ARRAY(J+1)
400    CONTINUE

C
C      REWIND TAPE

C
      A=3
      CALL MTAPEF(A,B)
      IF(B.NE.1)WRITE(6,160)B

C
C      DO A CLOSE

C
      A=16
      CALL MTAPEF(A,B)
      IF(B.NE.1)WRITE(6,170)B

C
C
100    FORMAT(' ','ERROR ',I3,' IN MAG TAPE INITIALIZE')
110    FORMAT(' ','ERROR ',I3,' IN MAG TAPE OPEN')
120    FORMAT(' ','ERROR ',I3,' IN MAG TAPE WRITE')
130    FORMAT(' ','ERROR ',I3,' IN SETTING FILE MARK')
140    FORMAT(' ','ERROR ',I3,' IN FIRST REWIND')
150    FORMAT(' ','ERROR ',I3,' IN MAG TAPE READ')
160    FORMAT(' ','ERROR ',I3,' IN SECOND MAG TAPE REWIND')
170    FORMAT(' ','ERROR ',I3,' ERROR IN MAG TAPE CLOSE')
      END

```

### CLOSEU (Close with Update) Subroutine

This subroutine closes a file with update and moves the current end sector to the current end of the file. This subroutine is written in assembler.

#### Form

CALL CLOSEU(1un)

where:

1un = Logical unit number associated with the file.

## System Subroutines

### CONCAT

### CONCAT

The CONCAT subroutine is used to concatenate character strings.

Form: CALL CONCAT (a, b, out(, len(, err)) )

Where:	a	is the array containing the left string
	b	is the array containing the right string.
	out	is the array into which the concatenated result is placed. This array must be at least one element longer than the maximum length of the result string (i. e. , one greater than the value of len, if specified).
	len	is the integer number of characters representing the maximum length of the output string. The effect of len is to truncate the output string to a given length, if necessary.
	err	is the Logical error flag set if the output string is truncated to the length specified by len.

The string in array "a" immediately followed on the right by the string in array "b" and a terminating null character replaces the string in array "out". Any combination of string arguments is allowed so long as "b" and "out" do not specify the same array. Concatenation stops either when a null character is detected in "b" or when the number of characters specified by "len" have been moved.

If whether the left or right string is a null string, the other string is copied to "out". If both are null strings, then "out" is set to a null string. The old contents of "out" are lost when this routine is called.

Errors:

Error conditions are indicated by "err", if specified. If "err" is given and the output string would have been longer than "len" characters, then "err" is set to .TRUE.; otherwise, "err" is unchanged.

Example:

The following example concatenates the string in array STR and the string in array IN and stores the resultant string in array OUT. OUT cannot be larger than 29 characters.

```
LOGICAL*1 IN(30), OUT(30), STR(7)
.
.
.
CALL CONCAT(STR, IN, OUT, 29)
```

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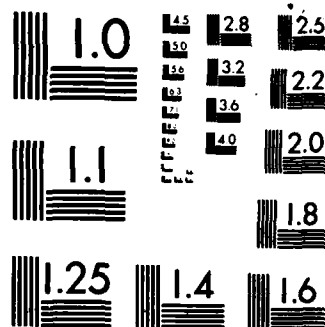
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```
.TITLE LUNDEF
.CSECT LUND
.MCALL EXEC
.MCALL RESTORE,SAVE,.REGDEF
.GLOBL LUNDEF
.REGDEF
LUNDEF: SAVE R0,R1,R2,R3,R4,R5
        TST (R5)+
        MOV (R5)+,R2
        EXEC CLIS,R2
        BCC RET
        MOV #1,0(R5)
        CLC
RET:     RESTORE R5,R4,R3,R2,R1,R0
        RTS PC
        .END
```

END

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